

## Z. Materials Simulation, Computation and Design

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### Z-01

#### **Large-scale GPU computations of dendrite growth using phase-field method**

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Phase-field method has emerged as a powerful tool for computing a complicated dendrite growth. Now, the phase-field method is accepted as the most accurate model to express the dendrite structure. Nevertheless, there are some unsolved issues for the phase-field method. One major issue is the large computational cost caused by the diffuse interface model. Although, thanks to the development of the quantitative phase-field methods [1], we could use a large computational lattice, the lattice size is also restricted by the characteristic length, such as the dendrite tip radius. In order to enable the large-scale phase-field simulations, we have been developing the parallel GPU computational schemes for the GPU supercomputer. Until now, we have performed the large-scale phase-field simulations of competitive dendrite growth during directional solidification of a binary alloy in single-crystal [2], bicrystal [3, 4], and polycrystal [5]. In this presentation, those large-scale phase-field simulations of dendrite growth are introduced.

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*Keywords: phase-field method, large-scale simulation, GPU, dendrite, competitive growth*

### Z-02

#### **Chemically selective alternatives to photoferroelectrics for polarization-enhanced photocatalysis: the untapped potential of hybrid inorganic nanotubes**

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**Objective:** In spite of the potential benefits for Sustainable Energy and Chemistry, integration of chemical separation and polarization-enhanced photo-catalysis into one solution based on cheap and scalable materials is yet to be realized. **[Methods]** Strategies to integrate chemical separation and polarization-enhanced photo-catalysis into hybrid organic-inorganic nanotubes (NTs) have been screened in silico by mean of linear-scaling Density Functional Theory (LS-DFT) and related perturbative approaches to optical absorption. **[Results]** The simulations elucidate the interplay between chemical functionalization, curvature, local permanent polarizations, band gap, band-separation, band-alignment and the occurrence of charge-transfer excitations in an existing class of hybrid organic-inorganic NTs with hydrophobic interior and hydrophilic exterior: methylated aluminosilicate imogolite NTs. Strategies based on the generated insight have been suggested to increase the NT polarization to values comparable with state of the art ferroelectric photo-catalysts, and to tune NT-reactant electronic alignments by altering the NT radius and wall-thickness. **[Conclusions]** LS-DFT simulations of existing methylated imogolite NTs suggest that integration of chemical separation and polarization-enhanced photo-catalysis into one material could be possible. Separate control of cavity electrostatics and polarization-enhanced electron-hole separation may enable implementation of innovative strategies based on the use of local-polarizations in overall dipole-free (chemically selective) NTs to force reactants to match the photocatalyst, as opposed to standard band-engineering of photo-catalysts for a given reactant.

*Keywords:* photocatalysis, ferroelectrics, chemical separation, hybrid inorganic nanotubes, linear-scaling density functional theory

### Z-03

#### Surface adhesion and its effect on new semiconductor technologies

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Many options for new semiconductor technologies involve self-assembly of 2D or 1D materials or functional molecules on surfaces. Typically weak van der Waals bonds hold such structures in place, determining structure, polymorphism, contact resistance, and transport properties. Also, strong van der Waals forces are often mis-interpreted as chemical bonds, confusing synthetic chemical and synthetic understanding. New methods and results are presented describing: [1] measurement and DFT-based calculation of free-energies of polymorphism of large alkylporphyrin self-assembled monolayers on graphite surfaces from organic solution, and [2] conceptual methods for understanding of sulfur-bound ligands to gold surfaces and nanoparticles, providing the first rational understanding of synthetic strategies and spectroscopic measurements. This is done inside a general discussion of modern a priori treatments of van der Waals forces in self assembly. These forces are not included in traditional GGA or hybrid density-functionals, limiting the application of high-level calculations to understand system structure and properties. Very simple approaches that treat the quantum-mechanical fluctuations driving the van der Waals force as being local and pairwise additive work well for interacting insulators or small molecules, although one needs to consider the chemical environment of the electrons to obtain quantitative accuracy. However, in larger systems involving conductors, many-body effects can become important, leading for example to dielectric screening of the van der Waals force. This effect produces one of the cancellations of errors that contributes significantly to the success of GGA methods in materials applications. In addition, van der Waals fluctuations in interacting 1D and 2D conductors may be of longer range than component spacings, greatly increasing the strength of the force.

*Keywords: DFT, dispersion, self assembly, gold thiolate, free energy*

#### **Z-04**

##### **Interfaces of 2D materials and oxides – first – principles studies**

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Two-dimensional (2D) materials such as graphene and 2D transition metal dichalcogenides (TMDs) have been extensively studied for electronic applications, due to their attractive electronic properties such as high mobility. In real device applications, however, it is necessary to integrate the channel materials with other materials. For example, based on the CMOS technology, a gate dielectric material, such as high dielectric constant (high-k) oxide is required, and the interface between the 2D material and the gate oxide is expected to play a crucial role in the performance of such devices. Using first-principles calculations based on the density functional theory (DFT), we have investigated the interfacial properties between graphene or 2D TMDs and various oxides such as HfO<sub>2</sub>, Al<sub>2</sub>O<sub>3</sub>, Y<sub>2</sub>O<sub>3</sub>, Si<sub>3</sub>N<sub>4</sub>. Our calculations predict that a monolayer of Y<sub>2</sub>O<sub>3</sub> can be formed on graphene with weak interfacial interaction via a physical deposition process. A planar Al<sub>2</sub>O<sub>3</sub> monolayer, with a direct band gap of 5.99 eV and thermal stability up to 1100 K, is predicted to be stable and its stability can be enhanced by substrates such as graphene. The band offsets between the Al<sub>2</sub>O<sub>3</sub> monolayer and graphene are large enough for electronic applications. In addition, the non-polar  $\beta$ -Si<sub>3</sub>N<sub>4</sub> (0001) surface is predicted to be an excellent support for high mobility single-layer and bi-layer graphene. The weak interaction between oxygen-terminated HfO<sub>2</sub> (111) and the MoS<sub>2</sub> monolayer leads to symmetric band offsets which are larger than 1 eV. The presence of oxygen vacancies in HfO<sub>2</sub> enhances the interfacial interaction significantly, leading to electron-hole puddles, larger effective masses, and localized midgap states in the MoS<sub>2</sub>. Some of these results will be discussed.

*Key word: 2D materials, oxides, interface, first-principles calculation*

#### **Z-05**

##### **Computational discovery and design of 2D materials for energy and electronics application**

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The discovery of graphene [1-2] has led to significant development of a new family of 2D materials including hexagonal boron nitride, silicene, phosphorene, borophene, metal dichalcogenides and metal oxides etc. Our recent research mainly focuses on (i) predicting new graphene-like 2D Dirac materials [3-4]; (ii) exploring the functionalization of 2D materials for energy conversion [5-6]; (iii) engineering 2D van der Waals type hetero-structures to achieve the combined electronic functionalities that are unavailable from the individual 2D material [7-9]; (iv) predicting stability, electronic, mechanical and optical properties in the experimentally less-explored 2D materials [10-12]. In this presentation, I will share our most recent research progress in relation to the above topics.

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*Keywords:* 2D materials, density functional theory, van der Waals heterostructure, hydrogen production, CO<sub>2</sub> reduction

## Z-06

### **Analytical modeling of steady-state interface fracture of elastic multilayered beams subjected to four-point bending**

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Objective: To derive the general closed-form solution for the steady-state interface energy release rate of notched multilayered beams subjected to four-point bending. The solution is applicable to elastic multilayered systems with any number of layers and cracking at any interface. [Methods] In this technique, a notch is cut at the middle of the multilayered beam through a number of layers to provide a point for the initiation of the interface crack under four-point bending. The steady-state interface energy release rate can be derived as a function of the configuration of the system, the location of the interface crack, and the applied moment required to result in steady-state interfacial cracking. The solution is built upon the previously developed analytical model for multilayered beams subjected to bending in which only three unknowns are involved in the model regardless the number of layers in the system. [Results] In the present work, the beam can have arbitrary number of layers and fracture can occur at any interface. Specific results are calculated for alternate layered systems to elucidate the essential trends of the dependences of the normalized steady-state interface energy release rate on the thickness ratio and the modulus ratio for each interface. [Conclusion] In conclusion, we derive the general closed-form solution for the determination of steady-state interface energy release rate of multilayered systems from four-point bending tests. Fracture can occur at any interface. We apply the solution to alternate bilayered, trilayered, and four-layered systems to elucidate the essential trends. The physical meanings of the trends of the dependences of the normalized steady-state interface energy release rate on the thickness ratio and modulus ratio are discussed for each location of the fractured interface.

*Keywords:* multilayer, bending test, layered structure, analytical method

## Z-07

### **Grand design of new electronic materials and properties**

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Discovery of new classes of materials with new functionalities or significantly improved performance has always been the driving force for the advance of modern science and technology, and the improvement of our daily lives. Searching for new class of materials with exotic properties has always been challenging because of the complexity of both the theoretical and the experimental approaches developed so far. This talk will present a number of new strategies we have developed for the design of new materials and properties. It is expected to show how complicated science and materials design could be made simple and enjoyable. A new concept, the codes of matter/materials based on the three ubiquitous and paramount attributes of all existing matter/materials, charge, spin, freedom of motion will be introduced. We will discuss the principles of the codes and their applications in material and property design. Many new types of materials with exotic properties and their possible experimental realizations will be discussed.

## **Z-08**

### **Topological semimetals: materials prediction by first-principles calculations**

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Topological semimetals, characterized by Weyl/Dirac nodes in the bulk and Fermi arcs on surface, are new states of three-dimensional (3D) quantum matters, as an extension of topological classification from insulators to metals. The low energy excitation in Dirac/Weyl semimetal is the same as the Dirac/Weyl equation used for describing the massless Dirac/Weyl fermion. The Weyl fermion has certain chirality and has not been discovered since Hermann Weyl proposed it in 1929. An interesting special case where the Dirac nodes or Weyl nodes forming a closed or continuous line in momentum space is also introduced. Such topological semimetal is so-called Node-Line Semimetal. In this talk, I will introduce our predictions of realistic materials to realize Dirac, Weyl and Node-Line semimetals. The experimental confirmation and discovery of 3D massless Dirac fermion and Weyl fermion are also discussed. At last, a kind of new massless fermion quasiparticles with triply degenerate nodal points will be introduced and the four members of topological semimetal family and their relationship are summarized.

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*Keywords: Topological semimetal, Dirac semimetal, Weyl semimetal, Node-Line semimetal*

## **Z-09**

### **Computational materials design: from a simple chemical concept to 3D topological materials**

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Within recent years, topological materials, including topological insulators, topological crystalline materials, topological (Dirac) semimetals, topological Weyl semimetals, topological Weyl line-node (or node-line) semimetal as well as topological metals, become extensively interesting not only for condensed matter physics and materials science but also for fundamental Dirac fermions. We have proposed a simple chemical consideration to design three-dimensional topological materials according to the electronegativity concept in combination with first-principles calculations. For instance, because the metal element of bismuth offers a very strong spin-orbit coupling effect and easily induces so-called band-inversion occurrence, which are significant for the non-trivial topological states, most of topological materials basically consist of bismuth in its  $\text{Bi}^{3+}$  valence state. From the viewpoint of chemical formation, in order to form a  $\text{Bi}^{3+}$  configuration in a topological material it will need other constituents having larger electronegativity than that of Bi, such as Se, Te, O, S, C, Pb, F, Cl, Br, I, etc. Within this situation, Bi lose its three p valence electrons in the form of the fully unoccupied Bi-p-orbits states. Of course, in some topological materials Bi also has its  $\text{Bi}^{3-}$  valence state, such as some antiperovskite TIs or TCIs. This negative valence state of Bi can be attributed to the fact that the electronegativity of the constituents (i.e., alkaline-earth and alkali elements) in a compound are much lower than that of bismuth and Bi would obtain three valence electrons to form its fully filled p orbits. In this presentation, we will summarize what we have obtained for computational design of 3D materials from topological insulators to 3D topological 3D Dirac semimetal to 3D Dirac node-line in pure metals.

*Keywords: topological materials, semimetals, Dirac and Weyl fermions, first-principles calculations*

## **Z-10**

### **Integrated microstructure modeling during transformation and deformation**

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The key to predicting, and therefore optimizing, properties of materials is the knowledge of the state of microstructure. In the past decade, unprecedented methods to quantify, use and explore grain- and precipitate-scale microstructures have been developed. However, most modeling approaches to microstructure-property relationship utilize highly simplistic descriptors of microstructures (such as average particle size and volume fraction) that are empirically correlated to the properties (e.g., cutting vs. looping). Such approaches are utterly inadequate for addressing the location-specific design needs. ICME will remain empirical data driven with limited predicting power and payoffs without the development of next generation modeling tools that incorporate specific transformation and deformation mechanisms operating in specific alloy systems under a given set of processing parameters, microstructure states and service conditions. In this presentation, we focus on what one could do at the mesoscale to address this difficult challenge. In particular, using structural materials as examples we demonstrate how to integrate mesoscale modeling with experimental characterization to bridge ab initio calculations and crystal plasticity (CP) simulations to (a) identify transformation / deformation mechanisms and quantify activation pathways, (b) provide “mechanism maps” and constitutive laws for (i) microstructure evolution and (ii) dislocation – microstructure interaction as function of alloy composition, thermomechanical history, temperature and loading condition, and (c) integrate image-based mesoscale microstructure modeling with image-based fast Fourier transform (FFT) CP for co-evolution of microstructure (precipitates, grains, cracks, voids, etc.) and dislocations in an RVE of continuum level FEM.

*Keywords: phase transformation, microstructure evolution, dislocation, deformation, phase field*

## **Z-11**

## Stability analysis of NdFe<sub>12</sub>-based compounds as promising high performance permanent magnet materials

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Recently, a series of the ThMn<sub>12</sub>-type compounds, NdFe<sub>12</sub>, NdFe<sub>12</sub>N, were predicted theoretically as the promising high performance permanent magnetic materials with the high magnetization and magnetocrystalline anisotropy energy which are comparable to the well known Nd-Fe-B magnets. However, these compounds are very difficult to be synthesized in the experiments due to the thermodynamic instability. The present study attempts to investigate the origin of the instability in several NdFe<sub>12</sub>-based compounds, to discuss the effect of Ti-doping on the stabilization of the NdFe<sub>11</sub>Ti and NdFe<sub>11</sub>TiN from the first-principles. Calculations of the electronic structure are based on GGA-PAW, +U are used for both Nd and Ti. The Debye-Gruneisen approximation, as well as the phonon calculations are performed to estimate the finite temperature properties. The calculations revealed that (1) The FeNd<sub>12</sub> has both thermodynamical instability and dynamic instability; (2) The vibration effect at finite temperature brings the possibility to stabilize the NdFe<sub>12</sub> at 620K; (3) The analysis and comparison of different features of the effective pair interactions in NdFe<sub>12</sub> and Ti-substitution NdFe<sub>12</sub> shows that introducing attractive pair interactions due to Ti-doping is one of reasons of the stabilization of NdFe<sub>11</sub>Ti; (4) the mixing energy of NdFe<sub>12</sub> and NdTi<sub>12</sub>, and the stable range of Ti-substitution have been evaluated, the system with the minimum mixing energy at the whole concentration range is NdFe<sub>11</sub>Ti, which is consistent with the experimental results.

*Keywords: stability, NdFe<sub>12</sub>, permanent magnets, first-principles*

### Z-12

#### Role of polar phonons in the photo excited state of metal halide perovskites

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**Objective:** The development of high efficiency perovskite solar cells has sparked a multitude of measurements on the optical properties of these materials. For the most studied methylammonium(MA)PbI<sub>3</sub> perovskite, a large range (6-55 meV) of exciton binding energies has been reported by various experiments. The existence of excitons at room temperature is unclear. We calculate the exciton binding energies by means of a fully ab-initio approach and study the effect of ionic screening on the exciton binding energy. **[Methods]** For the MAPbX<sub>3</sub> perovskites we report on relativistic Bethe-Salpeter Equation calculations (GW-BSE). This method is capable to directly calculate excitonic properties from first-principles. We use density functional perturbation theory and a novel method based on finite temperature molecular dynamics to calculate the dielectric function including both electronic and ionic contributions. **[Results]** At low temperatures our method predicts exciton binding energies in agreement with the reported large values. For MAPbI<sub>3</sub>, phonon modes present in this frequency range have a negligible contribution to the ionic screening. By calculating the polarization in time from finite temperature molecular dynamics, we show that at room temperature this does not change. **[Conclusions]** We therefore exclude ionic screening as an explanation for the experimentally observed reduction of the exciton binding energy at room temperature and argue in favor of the formation of polarons.

*Keywords: BSE, GW, excitons, dielectric function, perovskite solar cells*

## **Z-13**

### **Microscopic model study of strongly correlated 5d transition metal Ir oxides**

Seiji Yunoki

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Motivated by recent experiments of novel 5d Mott insulators in  $\text{Sr}_2\text{IrO}_4$ , we have studied theoretically the two dimensional three-orbital Hubbard model on the square lattice with a strong spin-orbit coupling. The variational Monte Carlo method and the dynamical mean field theory are used to obtain the ground state phase diagram with varying a on-site Coulomb interaction  $U$  as well as the spin-orbit coupling. It is found that the transition from a paramagnetic metal to an antiferromagnetic (AF) insulator occurs at a finite  $U = U_{\text{MI}}$ , which is greatly reduced by a large spin-orbit coupling, characteristic of 5d electrons, and leads to the “spin-orbit-induced” Mott insulator. It is also found that the Hund’s coupling induces the anisotropic spin exchange and stabilizes the in-plane AF order. We have further studied the single-particle excitations using the variational cluster approximation and the dynamical mean field theory, and revealed the internal electronic structure of this novel Mott insulator, i.e., the effective total angular momentum  $J_{\text{eff}}=1/2$  Mott insulator. We have estimated the magnetic exchange coupling and found that it can be as large as 50-100 meV. These findings are in agreement with experimental observations for  $\text{Sr}_2\text{IrO}_4$  and very similar to mother compounds for high  $T_c$  cuprate superconductors. It is therefore expected that a possibly high  $T_c$  superconductivity can be induced once mobile carriers are introduced into the  $J_{\text{eff}}=1/2$  Mott insulator. We have considered this possibility using the variational Monte Carlo method as well as RPA and found that indeed the superconductivity with d-wave pairing is most likely induced. We will also discuss the similarity in the single-particle excitations between iridates and cuprates, including pseudogap behavior, and other related systems. This work has been collaboration with H. Watanabe, T. Shirakawa, T. Sato, K. Nishiguchi, B. H. Kim, K. Seki, W. Fan, and H. Sakakibara. strongly correlated materials, 5d electrons, spin-orbit coupling.

## **Z-14**

### **Origin of the metal-insulator transition of indium atom wires on Si(111)**

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Low-dimensional electronic systems exhibit a number of exotic phenomena such as Peierls instability, magnetic ordering, superconductivity, Mott physics, or non-Fermi-liquid ground states. It is very challenging to understand such unique electronic properties in 1D and 2D electronic systems, which are fundamentally different from 3D cases. In this talk, I will present our recent density-functional theory studies for the origin of the insulating phases in the prototypical 1D electron system. As the first issue, the precise driving force of the phase transition in indium nanowires on Si(111) has been controversial whether it is driven by a Peierls instability or by a simple energy lowering due to a periodic lattice distortion. Unlike the conventional DFT calculations with the LDA and GGA, the present van der Waals (vdW) corrected hybrid density functional calculation [1] predicts that the low-temperature  $8 \times 2$  structure whose building blocks are indium hexagons is energetically favored over the room-temperature  $4 \times 1$  structure. We show that the correction of self-interaction error and the inclusion of vdW interactions play crucial roles in describing the covalent bonding, band-gap opening, and energetics of hexagon structures. The results manifest that the formation of hexagons occurs by a simple energy lowering due to the



lattice distortion, not by a charge density wave formation arising from Fermi surface nesting. Furthermore, our first-principles calculations demonstrate that the structural phase transition from the high-temperature 4x1 phase to the low-temperature 8x2 phase occurs through an exothermic reaction with the consecutive bond-breaking and bond-making processes, giving rise to an energy barrier between the two phases as well as a gap opening [2]. This atomistic picture for the phase transition not only identifies its first-order nature but also solves a long-standing puzzle of the origin of the metal-insulator transition in terms of the x2 periodic lattice reconstruction of In hexagons via bond breakage and new bond formation.

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## Z-15

### Jahn-Teller distortion in LiMn<sub>2</sub>O<sub>4</sub> and its effect on the lithiation process

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We performed extensive first-principles studies on the valence arrangement and magnetic configuration of the spinel-type LiMn<sub>2</sub>O<sub>4</sub>, a promising candidate of cathode materials in Li-ion batteries. The most stable LiMn<sub>2</sub>O<sub>4</sub> has an anti-ferromagnetic orthorhombic spinel structure, where Li atoms only occupy the octahedral center and Mn<sup>3+</sup> and Mn<sup>4+</sup> atoms occupy the tetrahedral and octahedral center, respectively. Different from the AFM ordering of Mn atoms along [110] or [001] direction in the literatures, we found that the Mn<sup>3+</sup> and Mn<sup>4+</sup> layers alternate along the [001] direction in the ground state of LiMn<sub>2</sub>O<sub>4</sub>. Hence the Jahn-Teller distortion causing from Mn<sup>3+</sup> atoms in LiMn<sub>2</sub>O<sub>4</sub> is relatively localized. The anti-ferromagnetic configuration we constructed here makes magnetization repulse effect weak, which is also good to the structure stability. We analyzed the diffusion pathway and energy barriers of Li ion in the most stable LiMn<sub>2</sub>O<sub>4</sub>. It was found that the Li ion diffuses through a ring consisting of six Mn atoms, but the valence of Mn atoms significantly affects the value of energy barrier. Our theoretical results may provide instructive information for the new design of high performance LiMn<sub>2</sub>O<sub>4</sub> cathode material.

*Keywords: Jahn-Teller distortion, LiMn<sub>2</sub>O<sub>4</sub>, cathode materials, first-principles studies*

## Z-16

### Two-dimensional materials goes to binary: Dirac cone formation in A<sub>x</sub>B<sub>4-x</sub> (A,B= C,Si,Ge, x= 1,3)

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Compared with monolayers consisting of single component, two-dimensional (2D) binary materials exhibit richer electronic structures associated with various atomic structures due to the varied composition and arranged pattern. Understanding the formation of Dirac cone (DC) band structures helps to design novel 2D electronic materials. As examples, AB<sub>3</sub> and A<sub>3</sub>B, A,B= C, Si, Ge were studied in this work utilizing tight-binding method parameterized by density functional calculations. The DC formation processes of SiC<sub>3</sub> and Si<sub>3</sub>C were analyzed and a “ring coupling” mechanism was proposed conceptually, extended further to understand DC formations in the binary C-Ge and Si-Ge 2D systems. The conditions of the system becoming self-doped were also discussed.

*Keywords: 2D materials, binary, Dirac cone, Density functional materials, Tight-binding model*

## **Z-17**

### **The role of Hubbard, dispersion and O<sub>2</sub> overbinding corrections for $\alpha$ -Fe<sub>2</sub>O<sub>3</sub> surface energy, magnetic ordering and band alignment**

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Objective: Sustainable molecular hydrogen generation using solar energy conversion can contribute to current energy needs. Hematite iron-oxide ( $\alpha$ -Fe<sub>2</sub>O<sub>3</sub>) is a promising photocatalytic anode material for hydrogen production, and improving the efficiency of hematite as a photo anode is an active area of research. In spite of this, best practice for its simulation via Density Functional Theory (DFT) is yet to be firmly established. To this end, here we benchmark the role of isotropic ( $U_{\text{eff}}$ ) vs anisotropic (U-J) Hubbard corrections, van der Waals terms, and O<sub>2</sub> over binding correction for the simulation of the material and its surfaces. [Methods] We have carried out DFT investigation of the structure, energy, electronic and magnetic properties of bulk hematite as well as of different  $\alpha$ -Fe<sub>2</sub>O<sub>3</sub>(001) surfaces by mean of subspace [ $U_{\text{eff}}$ , (U-J)] and dispersion corrected plane-wave DFT. [Results] Screening of different magnetic ordering for the bulk phase indicates Anti-Ferromagnetic (AFM) order to be energetically favored. AFM ordering is maintained in the bulk-region of sufficiently thick (001) slabs. The different approaches considered lead to minimally altered lattice parameter, surface energy, electronic and magnetic properties for sufficiently thick slabs. However, the surface energy and relative stability of different  $\alpha$ -Fe<sub>2</sub>O<sub>3</sub>(001) terminations are strongly sensitive to the inclusion of dispersion terms and corrections to the O<sub>2</sub> GGA overbinding error in the simulations. [Conclusions] The structural, electronic and magnetic properties of  $\alpha$ -Fe<sub>2</sub>O<sub>3</sub>(001) surfaces are minimally altered by using isotropic ( $U_{\text{eff}}$ ) and anisotropic (U-J) Hubbard corrections or dispersion terms. However, when accounting for the GGA-error in O<sub>2</sub> over-binding, significant changes occurs in the computed surface energies. At higher oxygen chemical potential, previously overlooked terminations with excess oxygen are become energetically favored over those with excess iron, as observed experimentally.

*Keywords: hematite, surface energy, Hubbard corrections, magnetic properties, photocatalysis*

## **Z-18**

### **Manipulating topological phases in honeycomb structure**

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Band topology of strained buckled honeycomb consisting of different elements (IV, V and III-V) as well as those placed on a variety of semiconducting and insulating substrates are systematically investigated using first-principles calculations [1-5]. Topological phase can be manipulated not only through strain but also through bonding with the supporting substrate and functionalization. The honeycomb can exhibit quantum spin Hall effect phase, topological crystalline phase, and quantum anomalous Hall effect phase. In addition, some metal induced reconstructed substrates can be 2D topological insulator. This opens up new opportunities for the scientists in the field of surface science.

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*Keywords: topological insulators, 2D materials, quantum spin Hall effect*

## Z-19

### Localized excitation of Ti<sup>3+</sup> ions in the photoabsorption and photocatalytic activity of reduced rutile TiO<sub>2</sub>

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In reduced TiO<sub>2</sub>, electronic transitions originating from the Ti<sup>3+</sup>- induced states in the band gap are known to contribute to the photoabsorption, being in fact responsible for the material's blue color, but the excited states accessed by these transitions have not been characterized in detail. In this work we investigate the excited state electronic structure of the prototypical rutile TiO<sub>2</sub>(110) surface using two-photon photoemission spectroscopy (2PPE) and density functional theory (DFT) calculations. Using 2PPE, an excited resonant state derived from Ti<sup>3+</sup> species is identified at 2.5±0.2 eV above the Fermi level (E<sub>F</sub>) on both the reduced and hydroxylated surfaces. DFT calculations reveal that this excited state is closely related to the gap state at ~ 1.0 eV below E<sub>F</sub>, as they both result from the Jahn-Teller induced splitting of the 3d orbitals of Ti<sup>3+</sup> ions in reduced TiO<sub>2</sub>. Localized excitation of Ti<sup>3+</sup> ions via 3d→3d transitions from the gap state to this empty resonant state increases significantly the TiO<sub>2</sub> photo-absorption and extends the absorbance to the visible region, consistent with the observed enhancement of the visible light induced photocatalytic activity of TiO<sub>2</sub> through Ti<sup>3+</sup> self-doping. Our work reveals the physical origin of the Ti<sup>3+</sup> related photoabsorption and visible light photocatalytic activity in prototypical TiO<sub>2</sub>, and also paves the way for the investigation of the electronic structure and photoabsorption of other metal oxides.

*Keywords: TiO<sub>2</sub>, catalysis, transition state*

## Z-20

### Quantitative phase-field modeling and simulations of competitive growth of dendrites in alloy systems

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Control of solidification microstructure of alloys is one of important subjects in the field of metallurgy because the size and morphology of the solidified crystals and non-uniform distribution of alloying elements, i.e., microsegregation determine the quality of as-cast materials. The alloy solidification by its nature is a multi-physics problem involving fluid dynamics, thermal and solute diffusion and so on. Hence, analyses of the

formation processes of solidification microstructures require these physics and their coupling to be explicitly taken into account. The phase-field model has emerged as an effective computational tool for simulating microstructural evolution processes in multi-physics problems. In this diffuse interface approach, one can avoid explicitly tracking the position of interface in complex microstructural patterns, which is the chief advantage of this model. Although the early-developed models have a serious shortcoming regarding the quantitative accuracy, so-called quantitative phase-field model now enables us to carry out quantitative description and prediction of microstructural evolution processes. The quantitative phase-field model is formulated on the basis of the thin-interface asymptotics and it exactly recovers the sharp-interface equations of the free-boundary problem. This quantitative model was developed for solidification in pure substances and the alloy systems without diffusion in the solid phase. It was extended by our group to deal with isothermal solidification in binary alloy systems with diffusion in the solid and also non-isothermal solidification in multicomponent alloys with diffusion in the solid. Hence, this model is applicable to analyses of a number of important phenomena involving diffusion in the solid, such as the formation of microsegregation and peritectic reaction process. In this talk, our recent progress in the quantitative phase-field modelling and its application to investigation of competitive growth of dendrite in alloy systems are introduced in detail.

*Keywords: phase-field model, solidification, dendritic growth*

## **Z-21**

### **A quantitative and efficient phase-field model with finite interface dissipation and its application in materials science**

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A phase-field model with finite interface dissipation for the description of various phase transformations in multicomponent materials ranging from equilibrium state to strongly non-equilibrium state was first developed. In order for a further quantitative phase-field simulation of microstructure evolution during various materials process, especially for solidification, an anti-trapping current scheme considering diffusion in both liquid and solid phases was added in the phase-field model with finite interface dissipation. A careful asymptotic analysis indicated that for arbitrary solid diffusivity the proposed anti-trapping current term can eliminate all anomalous interface effects. Moreover, a novel approach was also developed to directly incorporate the general sublattice models in the CALPHAD formalism into the phase-field formalism for providing accurate energy and driving force information. Internal minimization of sublattice occupancy and solute evolution during microstructure transformation leads, in general, to a solution superior to the separate solution of the individual problems. In addition, a locally one-dimensional (LOD) semi-implicit scheme was proposed to improve the numerical efficiency of the phase-field simulation. With the LOD splitting, the multi-dimensional parabolic problem can be approximated numerically by individual treatment of the spatial variables in a single cycle. Each spatial variable can be treated in either real or Fourier space depending on the boundary conditions. The numerical tests indicated that the LOD semi-implicit scheme has noticeable advantages on the computational efficiency and accuracy in comparison with the traditional explicit or implicit schemes. The established quantitative and efficient phase-field model with finite interface dissipation was finally applied to quantitatively simulate the microstructure evolution during various materials process, and several typical examples were presented.

*Keywords: phase-field modeling, microstructure, CALPHAD, numerical scheme*

## **Z-22**

## **Prediction of the equivalent elastic modulus of mush zone during solidification process coupled with phase field simulations**

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The phase-field model is becoming a powerful tool to describe the complex interface pattern evolutions. It describes the microstructure using a set of conserved and non-conserved field variables that are continuous across the interface regions. A phase field model with the consideration of applied and thermal stress is developed in this paper. The elastic stress and strain fields inside the solid skeleton can be calculated out by phase field model together with the phase morphologies. By adding an external constant stress boundary condition, the total strain can be obtained by solving the mechanical equilibrium equations, which is a mechanical response to the external small applied stress. We can get the equivalent elastic modulus under different phase morphologies from these calculations, which is useful for FEM or FDM simulations on a larger scale. This model is applied to as-cast and semi-solid casting process, respectively.

*Keywords: phase-field model, equivalent elastic modulus, solidification, microstructure*

### **Z-23**

#### **Irradiation-induced void evolution in iron: a phase-field approach**

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Motivated by considering the thermodynamic parameters of material in conjunction with temperature, a serious computational data from ab initio molecular simulation is used to model the microstructure evolution of iron under irradiation using phase field method. The predicted void features including shape, size and density are in reasonable with the experimental observation. The morphology of saturated void in the irradiated microstructure under various temperatures is simulated. At the same irradiation temperature, there is an increment in the number of irradiated void with increasing dosage. While at the same dosage, there is a decrement in the number of void with increasing temperature. In order to further analysis the temperature and dosage effect, the porosity and density of post-irradiated iron are predicted. The temperature dependence of void porosity shows the expected bell-shaped curve, which is characterized by a peak at a certain temperature. The void density monotonically decreases with increasing temperature and increases with increasing dosage.

*Keywords: irradiated material, void evolution, phase field method, ab initio molecular dynamics*

### **Z-24**

#### **Design considerations of negative-stiffness composite materials for extreme viscoelastic and coupled-field properties**

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Objective: Effective viscoelastic and coupled-field properties, such as dielectricity and piezoelectricity, of composite materials may be greatly enhanced by negative-stiffness inclusions. However, in order to obtain such an extreme composite, considerations of the inclusion volume fraction, inclusion shape, inclusion electric conductivity and other factors are required to make the material stable.[Methods] In addition to the theoretical methods used in studying composite materials, finite element numerical methods and phase-field modeling are adopted in this research to calculate effective properties of the composites and their stability. [Results] Negative stiffness can be obtained by the post-buckling of a column, or in the vicinity of ferroelastic transitions, such as barium titanate. By using the phase-field modeling with the Ginzburg-Landau-Devonshire potential, the negative-stiffness effects can be obtained in consistent with experimental findings, as well as the finite element analysis and composite theory with inclusion's modulus assigned to be negative. In principle, the volume fraction of inclusions need to be small for large effective properties. However, for material stability, moderately large inclusion volume fraction with electrically conductive inclusions may be stabilized enhanced thermal expansion coefficient. Inclusion shapes play a minor role in the linear responses of the negative-stiffness composites. [Conclusion] By triggering ferroelastic transition, one may induce negative-stiffness effects in the composite or polycrystalline systems. Through material design, negative-stiffness composites may be stabilized for one or more effective properties.

*Keywords: negative stiffness, composite materials, viscoelastic and coupled-field properties, finite element method, phase-field modeling*

## **Z-25**

### **Nanoscaled martensitic transition and its abnormal properties in shape memory alloys**

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By impurity doping in shape memory alloys (SMAs), we propose a mechanism that leads to nanoscaled martensitic transformation accompanying with unique properties across a wide temperature range. Computer simulations (phase field method) using the Landau theory of phase transformations and Khachaturyan's microelasticity theory are used. Our simulations predict the formation of randomly distributed nanosized, singlevariant martensitic domains and a generic "phase diagram" including all the strain states in NiTi SMAs, which agrees well with experimental measurements. These nanoscale martensitic domains are frustrated and cannot evolve into long-range-ordered, internally twinned structures (i.e. long-range strain ordering). Such a structural state is found to evolve gradually upon loading and unloading or heating and cooling across a wide temperature range with narrow hysteresis. Further simulations show that this nanoscaled martensitic transition can induce unique Invar and Elinvar properties. We established a new phase diagram including all strain states in SMAs and found that the physical origin of nanoscaled martensitic transition can be attributed to large lattice distortion caused by doped defects. Those unique properties (small hysteresis, Invar and Elinvar) can be attributed to the continuous transition characteristics.

*Keywords: martensitic transition, phase field, strain glass, defect, nanodomains*

## **Z-26**

### **Finite element analysis of the tensile properties of triangular unit cell lattice structure based on selective laser melting process**

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Objective: With the rapid development of selective laser melting (SLM) technology, fabrication of lightweight lattice structure is no longer an insurmountable task. However, the variations in detailed shapes and sizes of the struts in lattice structures are constrained by the manufacturing capability of SLM process. This limitation generates a significant challenge in realizing engineered lattice structure. In this paper, the mechanical behaviour of AlSi10Mg lattice structure built from triangular unit cell with different dimensions constrained by SLM process was investigated by finite element analysis (FEA) using ANSYS®. [Methods] The geometry of a lattice structure with triangular unit cell was created in Creo® using a method proposed by the authors. Two finite element modelling methods using solid and beam element in ANSYS® were compared in terms of modelling complexity and computational efficiency. Based on the output, the effective in-plane Young's modulus,  $E$ , in both orthogonal directions of the structure was firstly examined. Then the effects of the number of unit-cell layers in out-plane direction was studied by modifying the unit cell height,  $h$ . Finally the effects of strut dimensions (length,  $l$ , and thickness,  $t$ ) on the strength of lattice structure were explored. In all cases, the volume of the lattice structure was kept constant. [Results] Solid element was chosen for finite element modelling because of the complexity in contact definition and more time-consuming in building line-based lattice structure by beam element. FEA results show that there are no significant differences in tensile and compressive  $E$  in both orthogonal directions. The mechanical properties of the lattice structure are independently affected by shape parameters. For a given ratio  $t/l=1/4.5$ , when the number of layers increases from 2 to 6 (by decreasing  $h$ ), the relative density of the lattice structure gradually increases from 0.15 to 0.26, while  $E$  increases from 0.05 to 0.12 times of the Young's modulus of the solid material. When the values of  $h$  and  $t$  are fixed,  $E$  increases when  $t/l$  ratio increases, which meets the same results for the ratio  $h/l$ . [Conclusions] Solid element is a more efficient method in modelling of lattice structure as compared to beam element.  $E$  is not affected by the alignment of the triangular unit cell in both orthogonal directions, but determined by parameters of the unit cell. These conclusions based on FEA results are necessary to be validated by experiments in the future.

*Keywords: finite element analysis (FEA), tensile properties, unit cell, lattice structure, selective laser melting (SLM)*

## **Z-27**

### **Self-healing properties of nanocrystalline materials: a first-principles analysis of the role of grain boundaries**

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Understanding the self-healing mechanisms of defects in nanocrystalline materials is of particular importance for developing the structural materials that can support extended component lifetime under extremely hostile conditions in nuclear reactors. Since grain boundaries are prevalent in nanocrystalline materials, they must affect, to some extent, the overall self-healing properties and the resultant mechanical responses. In the present work,

first principles calculations are carried out to investigate the energetic landscape of point defects (i.e. self-interstitials, He-interstitials, and vacancies) induced by the irradiation damage and the kinetics of the self-healing process in the vicinity of grain boundaries (GBs) in copper, focusing on six symmetric tilt grain boundaries that vary in their energies. Our results indicate that the interaction of vacancies with the self-interstitial and He-interstitial loaded GBs is very sensitive to the GB character. The low-energy GBs are generally accompanied by a higher propensity of self-healing behavior, in which the inter-granular interstitials and intra-granular vacancies recombine with each other. The recombination process is proved to be regulated by two mechanisms: interstitial emission mechanism and vacancy mediated mechanism. For the low-energy GBs, the former mechanism demonstrates its efficiency in describing the atomic motion, while for the high-energy ones, the latter turns out to be superior. With the aid of these mechanisms, we conclude that the low-energy GBs are comparatively more radiation-resistant than the high-energy counterparts, which may shed light on the rational design of high-performance structural materials based on nanocrystalline alloys.

*Keywords: nanocrystalline Cu, grain boundary energy, defect annihilation, diffusion mechanism, first-principles calculations*

## **Z-28**

### **Theoretical study on ternary and quaternary semiconductors: chemical stability, defects and dopants**

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The search for new direct bandgap, earth abundant semiconductors for efficient, high-quality optoelectronic devices, photovoltaic and photocatalytic energy conversion has attracted considerable interest. One methodology for the search is to study ternary and multiterinary semiconductors with more elements and more flexible properties. Cation mutation such as binary→ternary→quaternary for  $\text{ZnSe} \rightarrow \text{CuGaSe}_2 \rightarrow \text{Cu}_2\text{ZnSnSe}_4$  and  $\text{ZnO} \rightarrow \text{LiGaO}_2 \rightarrow \text{Li}_2\text{ZnGeO}_4$  led to a series of new quaternary chalcogenide and oxide semiconductors with wide applications. Similarly, starting with GaN, ternary nitrides such as  $\text{ZnSnN}_2$  and  $\text{ZnGeN}_2$  have been designed and synthesized recently. However, quaternary nitride semiconductors have never been reported either theoretically or experimentally. Through a combination of the Materials Genome database with the first-principles calculations, we designed a series of quaternary nitride compounds I-III-Ge<sub>2</sub>N<sub>4</sub> (I=Cu, Ag, Li, Na, K; III=Al, Ga, In) following the  $\text{GaN} \rightarrow \text{ZnGeN}_2 \rightarrow \text{I-III-Ge}_2\text{N}_4$  mutation. Akin to  $\text{Li}_2\text{ZnGeO}_4$ , these quaternary nitrides crystallize in a wurtzite-derived structure as their ground state. The thermodynamic stability analysis shows that while most of them are not stable with respect to phase separation there are two key exceptions:  $\text{LiAlGe}_2\text{N}_4$  and  $\text{LiGaGe}_2\text{N}_4$ , which are stable and can be synthesized without any secondary phases. Interestingly, they are both lattice-matched to GaN and ZnO, and their band gaps are direct and larger than that of GaN, 4.36 and 3.74 eV respectively. They have valence band edges as low as ZnO and conduction band edges as high as GaN, thereby combining the best of GaN and ZnO in a single material. We predict that flexible and efficient band structure engineering can be achieved through forming GaN/ $\text{LiAlGe}_2\text{N}_4$ / $\text{LiGaGe}_2\text{N}_4$  heterostructures, which have tremendous potential for ultraviolet optoelectronics.

*Keywords: ternary and quaternary semiconductors, chemical stability, defects and dopants*

## **Z-29**

### **Two dimensional antiferromagnetic Chern insulator: NiRuCl<sub>6</sub>**

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The quantum anomalous Hall effect (QAHE) arising from spin-orbit coupling (SOC) shows voltage transverse to the electric current even in the absence of an external magnetic field. Although the fundamental principle of QAHE has been proposed in a honeycomb lattice model [1] long ago, only latest experiment proves that the QAHE can be realized in Cr-doped  $\text{Bi}_2\text{Se}_3$  [2]. The direct approach to realize QAHE is to introduce FM order in quantum spin Hall insulators (QSHI) to break its time-reversal symmetry and turn its helical edge states to chiral ones. Such approach requires Chern insulator, or ferromagnetic (FM) insulator with a non-zero Chern number. Unfortunately, finding FM Chern insulator is very challenging because there are few ferromagnetic insulators in nature. As mentioned above, to archive QAHE, researchers pay more attentions to break the time reversal symmetry of topological insulator by importing ferromagnetic order. This reality easily allows people produce illusion that QAHE must connect with ferromagnetism. In the present work, by taking two dimensional transition metal halides (TMHs) as prototype model, we prove that QAHE can be realized in AFM material as long as the material shows spin-polarization and its time reversal symmetry is broken. The 2D TMHs mainly composed of transition metal atoms and halogen atom with the general formula  $\text{MnYm}$ , where M is a transition metal and X is halogen element (Cl, Br and I). To produce spin-polarization, we construct a new type 2D TMHs of  $\text{M}_1\text{M}_2\text{Y}_6$ , where the  $\text{M}_1$  and  $\text{M}_2$  represent 3d and 4d TM atoms, respectively, and Y is Cl. Our results indicate that under 5% compress strain in plane the single layer  $\text{NiRuCl}_6$  is 2D AFM QAHE insulator, or AFM Chern insulator.

*Keywords: antiferromagnetic Chern insulator*

### Z-30

#### **Orbital-lattice design for novel electronic devices and topological quantum phases based on conventional semiconductor surface**

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Objective: To design novel electronic devices and topological quantum phases that are in compatible with current semiconductor-based technology. [Methods] A combination of various theoretical approaches, including density functional theory based first-principles calculation, non-equilibrium Green's function method, ab initio molecular dynamics, effective Hamiltonian tight-binding modeling in together with Wannier function analyses, are employed for the research. [Results] We first study strain-engineered surface transport of Si(001), in order to isolate the surface states from bulk bands. Based on the finding, an ultrasensitive molecular sensor can be achieved by combining surface engineering and strain engineering. Also, the strain induced surface state isolation is used to realize ideal Rashba states on semiconductor surface, which can be used for the long-sought spin transistor. Then, we report conventional semiconductor (such as Si and Ge) based topological insulators with an extremely energy large gap of over 0.8 eV, which have great potential for room temperature applications. Last but not least, a novel 2D material,  $\text{sp}^2$  graphene is discovered. Compatible with Si-based technology, we found  $\text{sd}^2$  graphene also has many unique properties, with great potentials in physics, chemistry and materials science. [Conclusion] Importance of fundamental orbital-lattice design in determining the physical properties of new materials and devices for practical applications.

*Keywords: Orbital selection, lattice, topological quantum phase, semiconductor substrate, material design*

### Z-31

#### **RESCU: an electronic structure method for large systems**

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Objective: The major stumbling block for solving realistic materials problems is the lack of a first principles method that can efficiently and accurately simulate systems having many thousands of atoms. Well known packages of Kohn–Sham density functional theory (KS-DFT) can typically solve problems at a few hundred atoms level, and may solve slightly larger problems with supercomputers. Further approximations allows one to do better in computation at the expense of accuracy. There is an urgent need in finding novel computational mathematics that can overcome this stumbling block – in light of projects such as materials genome and atomistic TCAD. [Methods] RESCU (Matlab code) is a Kohn-Sham density functional theory (KS-DFT) solver by expressing Hamiltonian and electron wave-functions directly in real space grid, without any explicit basis sets. It is based on norm-conserving pseudopotentials (Troullier-Martins) and is designed for the ab initio quantum-mechanical calculations of the electronic properties of matter. Owing to the sparsity of the Hamiltonian matrix, the KS equations are solved by use of extremely efficient Chebyshev-filter technique. [Results] We demonstrate that RESCU can compute electronic structure for systems comprising many thousands of atoms using only modest computer resources, e.g. 16 to 256 cores. RESCU scales consistently as  $O(N^{2.3})$  from a few hundred atoms to about 8000 atoms with real space grids. The scaling is better or comparable in NAO basis up to the 14,000 atoms level. We solved KS-DFT for huge systems not possible before: a 5832 Si atoms supercell; a 8788 Al atoms supercell; a 5324 Cu atoms supercell; a small DNA molecule submerged in 1713 water molecules for a total 5399 atoms, etc.. The KS-DFT is entirely converged in just a few hours with the same accuracy as conventional KS-DFT solvers (e.g. VASP etc). In addition, problems of these sizes can be solved by RESCU on a single workstation having four K40 GPU cards. [Conclusion] Our results demonstrate that the RESCU method has reached a milestone of solving large scale materials simulation problems by KS-DFT on a modest computer cluster. I shall discuss further directions of RESCU developments and present the novel computational mathematics behind the huge efficiency gain.

*Keywords: Kohn–Sham density functional theory, Chebyshev-filter, real space*

## **Z-32**

### **Phase equilibria study of BaO-In<sub>2</sub>O<sub>3</sub>-B<sub>2</sub>O<sub>3</sub> system in B<sub>2</sub>O<sub>3</sub>-rich corner**

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Scintillators are materials which can efficiently absorb high energy radiation and transform it into radiation within or around the visible spectral region. In BaO-In<sub>2</sub>O<sub>3</sub>-B<sub>2</sub>O<sub>3</sub> system, Ba<sub>3</sub>InB<sub>9</sub>O<sub>18</sub> powders present an excellent scintillation property which makes it a good candidate for high energy detection. Therefore it is worth growing Ba<sub>3</sub>InB<sub>9</sub>O<sub>18</sub> crystal to make it practical since scintillators are usually crystal materials. Technological process of crystal growth needs the guidance of phase diagrams, while in BaO-In<sub>2</sub>O<sub>3</sub>-B<sub>2</sub>O<sub>3</sub> system this information is still limited. Under this circumstance, phase equilibria in B<sub>2</sub>O<sub>3</sub>-rich corner were studied. The thermal stability of Ba<sub>3</sub>InB<sub>9</sub>O<sub>18</sub> was studied through melting and quenching method, which melts peritectically into InBO<sub>3</sub> and liquid at about 1025°C. Isothermal sections at 900, 950, 1000, 1025, 1050°C in B<sub>2</sub>O<sub>3</sub>-rich corner were measured with EPMA and XRD, in which the boundary of liquid phase was determined by two constraint conditions (tie-line and Ba/In mole ratio). The primary crystal region of Ba<sub>3</sub>InB<sub>9</sub>O<sub>18</sub> was determined based on the established isothermal sections, which will be benefit to designing composition and process for crystal growth. Thermodynamic

assessment of this pseudo-ternary system was performed by CALPHAD method using Thermo-Calc software. The intermediate phases were treated as stoichiometric compounds and the liquid phase was described by the two-sublattice ionic liquid model. A set of self-consistent parameters was obtained and the calculation confirms well to the measurements. Due to the short of experiments, these parameters may only be valid in limited temperature and composition range.

*Keywords: BaO-In<sub>2</sub>O<sub>3</sub>-B<sub>2</sub>O<sub>3</sub> system, isothermal section, thermodynamic calculation, CALPHAD*

### Z-33

#### **Single-layer MS<sub>2</sub> nanoclusters: periodical structure and electronic property**

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Magic numbers exist for kinds of nanocluster formed by atoms or molecules, by which, the clusters are exceptionally stable. Here we report for the first time through a detailed theoretical investigations that the magic period of 3 for edge structures of the 2D transitional metal dichalcogenides. We find that the edge structure and energy gaps of triangular MoS<sub>2</sub> and WS<sub>2</sub> monolayer change periodically with the size of cluster. Specifically, the number of metal atoms per edge changes by 3, Fermi level crosses the top of conduction band, crosses the top of valence band, locates in the middle of band gap, which gives the metallic, metallic, semiconducting electronic property of MoS<sub>2</sub>/WS<sub>2</sub> nanoparticles every period of 3. However, metallic character of VS<sub>2</sub> nanocluster does not change with size, so does its ferromagnetism. Additionally, this kind of periodical change of atomic structures and energy gaps does affect their catalytic activity toward the hydrogen evolution reaction.

*Keywords: transitional metal dichalcogenides, morphology, edge-structure, period, catalytic activity*

### Z-34

#### **Room-temperature ordered spin structures in cluster-assembled single V@Si<sub>12</sub> sheets**

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Since most of the existing pristine two-dimensional (2D) materials are either intrinsically nonmagnetic or magnetic with small magnetic moment per unit cell and weak strength of magnetic coupling, introducing transition metal atoms in various nanosheets has been widely used for achieving a desired 2D magnetic material. However, the problem of surface clustering for the doped transition metal atoms is still challenging. Here we demonstrate via first-principles calculations that the recently experimentally characterized endohedral silicon cage V@Si<sub>12</sub> clusters can construct two types of single cluster sheets exhibiting hexagonal porous or honeycomb-like framework with regularly and separately distributed V atoms. For the ground state of these two sheets, the preferred magnetic coupling is found to be ferromagnetic due to a free-electron-mediated mechanism. By using external strain, the magnetic moments and strength of magnetic coupling for these two sheets can be deliberately tuned, which would be propitious to their advanced applications. More attractively, our first-principles molecular dynamics simulations show that both the structure and strength of ferromagnetic coupling for the pristine porous

sheet are stable enough to survive at room temperature. The insights obtained in this work highlight a new avenue to achieve 2D silicon-based spintronics nanomaterials.

### **Z-35**

#### **Thermoelectric properties of SnSe: understanding and pressure tuning**

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In the important widely-studied class of thermoelectric materials, it has been long standing problem to improve the energy conversion efficiencies. A simple layered binary compound, SnSe, free of Pb and expensive Te, was reported having the record breaking thermoelectric figure of merit  $ZT$  ( $> 2.6$ ) due to the ultralow lattice thermal conductivity. Using the First-principle Debye-Callaway approach, we simulate its lattice thermal conductivity, which in a reasonable agreement with the experimental measurement. The origin of the intrinsically ultralow lattice thermal conductivity of SnSe is understood based on elastic properties. The theoretical calculations and experimental measurements result that SnSe exhibits the low sound velocity and Young's modulus, indicating weak atomic interactions and strong lattice anharmonicity. However, the good thermoelectric properties of SnSe were achieved only at high temperature (923K), which limits the wide range usage of the compound. We illustrate how SnSe under pressure is an avenue to improve the thermoelectric properties of low-T SnSe phase (Pnma). The pressure-induced thermoelectric property enhancement of SnSe is mostly due to the pressure modified electronic structures of the compound.

*Keywords: DFT, thermoelectrics*

### **Z-36**

#### **The correlation between uniaxial negative thermal expansion and negative linear compressibility in $\text{Ag}_3[\text{Co}(\text{CN})_6]$**

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Density functional theory (DFT) calculations are used to investigate the correlation between the uniaxial negative thermal expansion (NTE) and negative linear compressibility (NLC) behaviors in  $\text{Ag}_3[\text{Co}(\text{CN})_6]$ . First, we reproduce the uniaxial-NTE and NLC behaviors under temperature- and pressure-field. And then the temperature dependence of elasticity is studied. The abnormal nature of elastic constants  $C_{33}$  and  $C_{11}+C_{12}$  as the function of temperature is predicted. The hardening of phonon modes (below  $564 \text{ cm}^{-1}$ ) with increasing temperature can be as an indicative for abnormal physical properties of  $\text{Ag}_3[\text{Co}(\text{CN})_6]$ . Through analyzing the vibration mode with the strongest phonon hardening, the deformation of wine-rack motif in anisotropic framework can be identified as the mechanism that leads to the coexistence of uniaxial-NTE and NLC in  $\text{Ag}_3[\text{Co}(\text{CN})_6]$ . The response of phonon group velocity along c-axis is intense and quicker than that of a-axis on heating and on compression, facilitating c-axis itself to be the carrier of abnormal uniaxial-NTE and NLC properties.

*Keywords: negative thermal expansion, negative linear compressibility, wine-rack motif*

### **Z-37**

#### **Effects of doping atom on the structural stability, mechanical and electronic structure of $\text{Mg}_2\text{Sn}$ phases from first-principles calculations**

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Using first-principles calculations based on density functional theory, the structural stability, mechanical and electronic structure of  $Mg_2Sn$  in anti-fluorite structure under element doping are investigated. Our results for the equilibrium structural parameters are consistent with the previous experimental and theoretical data. In this paper, we investigated the effects of Al, Zn, Ag or Zr doping on structural stability, mechanical properties and electronic structures of  $Mg_2Sn$  phases. We determined structural stability and mechanical stability of the doping phases and compared the influences of different doping ions on mechanical properties of  $Mg_2Sn$  phases. Meanwhile, we calculated the band structures, density of states and ionic configuration of doping phases to study their metallicity and ionic property. Based on the Poisson's ratio, the elastic constants, elastic modulus and the anisotropy was calculated. It is found that doping atoms has a significant effect on elastic properties due to form the metallic bond between atoms. In addition, When Al atoms instead of Mg atoms, Plastic is in the best of  $Mg_2Sn$  phase. Finally, analysis obtained atom doping doesn't change the metallicity of  $Mg_2Sn$  phase. From the figures of density of states, we found that the density of states in low energy area of  $Mg_2Sn$  phase increased after atom doping. There are orbital hybridization in  $Mg_2Sn$  and its doping phases, which implies that there exists covalent bonding in these phases.

*Keywords: magnesium alloys,  $Mg_2Sn$  phases, elements doping, structural stability, electronic structure*

## Z-38

### First principles investigations of two-dimensional transition metal carbides (MXenes)

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Two-dimensional (2-D) transition metal carbides  $M_{n+1}X_n$ s labeled as MXenes derived from ternary transition metal carbides MAX ( $M_{n+1}AX_n$ ) phases attract increasing attention due to their promising applications as Li-Ion battery anodes, hybrid electro-chemical capacitors and electronic devices. Experimentally, most MXenes are synthesized by chemical extraction of "A" layers from MAX phases. So far, MXene is the largest family of 2-D materials as there are more than 70 MAX phases available, hence the conventional route of synthesis-property characterization to obtain desirable MXenes is time-consuming and cost-demanding. In the present work, by performing systematic ab initio calculations and ab initio molecular dynamics simulations, we have unraveled the microscopic mechanism of forming MXenes from MAX phases and demonstrated the possibility and microscopic process of mechanical exfoliating 2D  $M_2C$  from  $M_2AlC$  phases; we have also shown that 2D  $Ti_{n+1}C_n$  are good candidates for flexible electron devices, and the mechanical failure of MXenes under tension is due to the elastic instability induced by collapse of the surface metal layer, while surface functionalization could slow down the collapse, resulting in striking increase of the critical strain of MXene;  $Cr_2C$  MXene is a half-metallic ferromagnet with a large gap of 2.85 eV, and the surface functionalization can induce the ferromagnetic (FM) to antiferromagnetic (AFM) transition in  $Cr_2C$  MXene accompanied by the metal to insulator (MIT) transition, where the surface functionalization induced localization of Cr d orbitals is responsible for the FM-AFM and MIT transition; our systematic ab initio calculations have also demonstrated that 2D  $Zr_2CO_2$  and  $Hf_2CO_2$  are potential photocatalysts for water splitting, showing very good optical absorption in visible light and good stability. Our results highlight the potential applications of MXenes in the spintronics and flexible electronics and photocatalysis.

*Keywords: ab initio calculations, MXenes, ab initio molecular dynamics simulations*

## **Z-39**

### **Growth, defects, oxidization, metal intercalation, and substrate effects of silicene**

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Silicene, a silicon analogue of graphene, has attracted increasing attention during the past few years [1]. Using first-principles calculations, we investigate the growth behavior of silicene on Ag(111) surface and explain the superiority of Ag substrate for silicene growth [2]. We also investigate the structures, formation energies, migration behaviors and electronic/magnetic properties of typical point defects in silicene, including the Stone-Wales defect, single and double vacancies, and adatoms [3]. In addition to the freestanding silicene, all these defects in (4×4) and (13×13)R13.9 silicene superstructures on Ag(111) surface are explored and compared with experimental STM images [4]. We propose that intercalation of potassium in bilayer silicene can effectively decouple the interaction between two silicene layers and recover the Dirac cones with a small band gap of 0.27 eV below the Fermi level [5]. The oxidization behavior of monolayer silicene in three typical phases are investigated and compared with experimental STM/STS measurement [6]. Moreover, we demonstrate a quasi-free-standing silicene layer through oxidization of bilayer silicene on the Ag(111) surface [7]. We also examine the electronic properties of silicene sheets on two kinds of representative inert substrates, i.e., hexagonal boron nitride (h-BN) monolayer and 4H-SiC(0001) surface [8]. Finally, we will briefly illustrate our recent results on germanene. Our theoretical results provide comprehensive guides of how to synthesize high-quality silicene and tailor its electronic properties.

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*Keywords: silicene, oxidization, defect, substrate*

## **Z-40**

### **The stability, edge reconstruction, and substrate selection of black phosphorene**

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Phosphorene, the monolayer of black phosphorus that was mechanically exfoliated in 2014, possesses many unique properties that are advantageous in electronic and optoelectronic device applications beyond graphene and TMDs. Using First-principles calculations, we indicated the substrate plays a critical role in the epitaxial growth of phosphorene. With compelling ab initial molecular dynamic simulations, it is found that phosphorene growth can only achieved on substrates with moderate (i.e., neither too weak nor too strong) substrate-phosphorene interaction. This criterion for a substrate suitable for phosphorene growth provides important guidelines for

experimental synthesis. Besides, a novel zz edge reconstruction of phosphorene with low energy and low barriers is disclosed, which is topologically distinctively different from any previously reported edge reconstruction. The reconstructed edge may be the dominant edge at room temperature in vacuum condition or even under low hydrogen gas pressure. Importantly, the calculated electronic properties are consistent with recent experimental measurements. It is expected that this newly found edge structure may spark a re-visit to the various properties of finite-size phosphorene, and further exploring their practical applications.

*Keywords: phosphorene, substrate, stability, edge reconstruction*

## Z-41

### Two-dimensional B-C-O alloy for electronics

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Graphene, a superior 2D material with high carrier mobility, has its limitation in the electronic devices due to zero band gap. In this regard, boron and nitrogen atoms have been integrated into the graphene lattice to fabricate 2D semiconducting heterostructures. It is an intriguing question whether oxygen can, in replacement of nitrogen, enter the sp<sup>2</sup> honeycomb lattice and form stable B-C-O monolayer structures. Here we explore the atomic structure, energetic and thermodynamic stability, and electronic properties of various 2D B-C-O alloys using first-principles calculations. Our results show that oxygen can be stably incorporated into the graphene lattice by bonding with boron. The B and O species favor alternately patterning into the chain- or ring-like structures embedded in the pristine graphene regions. These B-C-O hybrid sheets can be either metals or semiconductors depending on the B:O ratio. The semiconducting (B<sub>2</sub>O)<sub>n</sub>C<sub>m</sub> and (B<sub>6</sub>O<sub>3</sub>)<sub>n</sub>C<sub>m</sub> phases exist in the B- and O-rich conditions, and possess tunable band gap of 1.0~3.8 eV and high carrier mobility, retaining ~1000 cm<sup>2</sup>V<sup>-1</sup>s<sup>-1</sup> even for half coverage of B and O atoms. These B-C-O alloys form a new class of 2D materials as promising candidate for the high-speed electronic devices.

*Keywords: graphene, boron, oxygen, mobility, band gap*

## Z-42

### Iron carbides across dimensionality

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The study of iron carbides has been of great interest in recent years for its multiple applications from materials (magnetic, steel etc.) to catalysts (for carbon nanotube synthesis and Fischer-Tropsch synthesis etc.). Unfortunately, in the last decade, most of pioneers used surface/slab models or bulks to theoretically explain the behaviors of iron carbides. Indeed, the bulk and surface models and structures are easier to handle than cluster models. However, it is essential to explore the iron carbides across all dimensions to have deep understanding. Here, we extend the iron carbide system to clusters to understand the properties. In details, we perform a systematic comparison on the geometric, electronic, magnetic, thermodynamic properties of iron carbide clusters, including Fe<sub>x</sub>C<sub>y</sub> (x = 1~8, y = 1~8) and Fe<sub>2n</sub>C<sub>n</sub>, Fe<sub>5m</sub>C<sub>2m</sub>, Fe<sub>3n</sub>C<sub>n</sub>, Fe<sub>4m</sub>C<sub>m</sub> (m = 1~5, n = 1~7) predicted by Basin Hopping structure search algorithm + Density Functional Theory. We point out that iron-riched iron carbide clusters intends to be close packed with carbon atoms around the surface to form C<sub>2</sub> dimmers or C singles, while carbon-riched clusters intends to form long carbon chains. More important, we provide the reliable

thermodynamic stability diagrams for the iron-CO-CO<sub>2</sub>-Fe<sub>x</sub>C<sub>y</sub> system under different reaction conditions. In addition, the 2D iron carbides are predicted first, and are further confirmed in our surface experiment. The size and dimensional effect is discussed, which is important to rational design for iron-based catalysts and materials.

#### Z-43

##### **Single-spin manipulation by electric fields and adsorption of molecules**

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Magnetic anisotropy (MA), one of the most important parameters toward the ultimate limit of future data-storage systems single-atom memory, defines the thermal stability of the spin and the energy needed to switch it from one orientation to another one. Large MA is highly desirable for a stable and robust data storage against thermal fluctuation, but at the same time it makes the reversal of magnetization difficult. Therefore, systems with a large MA and easily controlled magnetization switching are in great demand. Performing ab initio calculations, we reveal that the magnetic anisotropy (MA) and the spin direction of a single adatom can be manipulated with a combination of electric fields and adsorption of molecules. Choosing the Fe adatom on the Cu<sub>2</sub>N/Cu(001) surface as a typical model system, we show that the MA of the pristine Fe adatom and the Fe adatom with an additional H or F atom adsorption remarkably changes by applying an external electric field. Moreover, we show that the F adsorption leads to the spin-reorientation transition of the Fe adatom from in plane to out of plane.

*Keywords: magnetic anisotropy, electric fields, molecule adsorption, density functional theory*

#### Z-44

##### **Application of first-principles computation on lithium-sulfur battery cathode design**

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Rechargeable lithium batteries are widely used in many applications owing to their high energy density, long lifetime and lightweight design. However, the current electrodes in consumer electronics market possess a limited theoretical specific capacity (~300 mAh/g), which cannot fulfill the increasing energy demands of modern society. Sulfur has the theoretical specific capacities of 1673 mAh/g, and meanwhile, with low cost and toxicity, which makes them attractive for commercial applications. Despite the considerable advantage, the successful implementation of lithium-sulfur batteries has been hindered by a series of obstacles, including poor cycle life, low Coulombic efficiency and low active material utilization. One of the main issues lies in the uncontrolled dissolution and loss of intermediate lithium polysulfide species into the electrolyte. Recently, there have been exciting developments in promoting the performances by introducing nano-structured additives, which can efficiently trap soluble lithium polysulfide during charge or discharge processes. Due to lack of microscopic insight into the interaction features between AM and Li<sub>2</sub>S<sub>n</sub> species, the choice of AM to use is largely empirical in nature. The theoretical study on the interactions inside cathode material system should be carried out, which is very important to understand the fundamental mechanism in atomic level, and provide the pathway for the further optimization of lithium-sulfur battery's performance. Using ab-initio computation scheme, the nano-material systems in cathode have been systematically investigated [1-3]. The studies focus on the interaction between lithium-sulfur species and cathode materials, in order for lithium-sulfur battery cathode design and performance optimization, and meanwhile, reveal the interaction mechanism in the cathode material system by analyzing electronic structure.



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*Keywords: lithium-sulfur battery, cathode design, anchoring material, ab initio computation*

## **Z-45**

### **Regulating mechanisms of electrochemical and chemical reactions in metal-oxygen and Li-ion batteries**

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There are very complicated electrochemical and chemical reactions occurred in charge and discharge processes in metal-oxygen and Li-ion batteries. Regulation of these reactions is an important strategy to optimize electrochemical performance by changing discharge products and charge reaction mechanisms. First-principles thermodynamics calculations combining with experimental verifications were performed to unravel regulating mechanisms of electrochemical and chemical reactions in metal-oxygen and Li-ion batteries. In this talk, several examples such as Li-O<sub>2</sub>, Na-O<sub>2</sub>, Li-ion cathode, and solid-state electrolyte materials were taken to present possible regulating mechanism in order to improve electrochemical performances of reducing overpotential and improving cycling stability. Our calculations reveal surface-acidity-dependent catalytic activity in reducing overpotentials of Li-O<sub>2</sub> batteries, electrolyte-controlled discharge product distribution in Na-O<sub>2</sub> batteries, and discharge-voltage-dependent structural evolution in Li-ion cathode materials. Our calculated predictions were further confirmed by our comparative experiments.

*Keywords: first-principles calculations, li-ion batteries, metal-O2 batteries, electrochemical reaction mechanisms*

## **Z-46**

### **Electronic structure calculations on the energetics of impurity atoms in Plutonium oxides**

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Plutonium (Pu) has been considered the most complicated and mysterious element in the Periodic Table because it exhibits many unusual physical and chemical properties rooted from its extremely complex 5f electronic states. Modern days problems regarding Pu involve in understanding its complex properties and predicting its aging. Among them, the solid-state properties and reaction behaviors of Pu oxides are the major concerns. However, taking solid-state properties for examples, available results focus on the two typical stoichiometric oxides, i.e., PuO<sub>2</sub> and Pu<sub>2</sub>O<sub>3</sub>. Very limited results have been reported on the behaviors of impurity atoms in PuO<sub>2</sub> and Pu<sub>2</sub>O<sub>3</sub>. From the point of view of applications, impurity atoms may play important roles in the solid-state properties and reaction behaviors of Pu oxides. In the presentation, the energetics of some typical impurity atoms (H, He, B, C, N, O, F, Ne, Cl, Ar, Kr, Xe and Ga) in PuO<sub>2</sub>, and two most-concerned impurity atoms (Ga and H) in Pu<sub>2</sub>O<sub>3</sub>, are calculated using a projector augmented-wave method under the framework of DFT+U. Three main incorporation sites for impurity atoms, i.e., octahedral interstitial, O vacancy, and Pu vacancy sites in both oxides, are considered. The results indicate that the energetics of impurity atoms depend significantly on the incorporation sites and on atomic properties such as atomic radius and electron affinity. Almost all impurity atoms considered

here are energetically unfavorable at the three incorporation sites, with the exception of the F atom at the octahedral interstitial and O vacancy sites in PuO<sub>2</sub>. The trends of incorporation energies of rare gas atoms generally reflect a size effect. Charge-transfer analysis reveals that the valence electrons can be polarized more easily with increasing atomic number of rare gas elements. The energetics of Ga in the two oxides show that the distribution of Ga in the Pu oxide layers is strongly dependent on the distribution and the concentration of Pu vacancy. On the whole, Ga concentration might decrease with the transitions of Pu → Pu<sub>2</sub>O<sub>3</sub> → PuO<sub>2</sub>. Additionally, the formation energies of hydrogen in UO<sub>2</sub> and PuO<sub>2</sub> show the different existence states of hydrogen: hydrogen in UO<sub>2</sub> energetically prefers to exist as a hydride ion ( $[(\text{UO}_2)_n]^+\text{H}$ ), whereas hydrogen in PuO<sub>2</sub> is relatively stable in the form of  $[\text{Pu}_n\text{O}_{2n1}]^+[\text{OH}]$ .

*Keywords: Plutonium oxides, crystal defects, Impurity atoms, density functional theory, electronic structure*

## Z-47

### **Pressure-driven 4f localized-itinerant transition in heavy fermion compound CeIn<sub>3</sub>: a first-principles many-body perspective**

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The localized-itinerant nature of Ce-4f valence electrons in heavy fermion compound CeIn<sub>3</sub> under pressure is studied thoroughly by means of the combination of density functional theory and single-site dynamical mean-field theory. The detailed evolutions of electronic structures of CeIn<sub>3</sub>, including total and partial density of states, momentum-resolved spectral functions, and valence state histogram etc., are calculated in a wide pressure range where the corresponding  $V/V_0 \in [0.6, 1.0]$  at T 116 K. Upon increasing pressure, two strong peaks associated with the Ce-4f states emerge near the Fermi level, and the c-f hybridization and valence state fluctuation are enhanced remarkably. Moreover, the kinetic and potential energies raise, while the occupancy, total angular momentum, and low-energy scattering rate of the Ce-4f electrons decline with respect to pressure. All the physical observables considered here exhibit prominent kinks or fluctuations in  $V/V_0 \in [0.80, 0.90]$ , which are probably the desired fingerprints for the Ce-4f localized-itinerant transition.

*Keywords: heavy fermion, dynamical mean-field theory, valence state histogram, localized-itinerant transition*

## Z-48

### **Density-functional study of plutonium monoxide monohydride**

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Plutonium monoxide monohydride (PuOH) is a potentially reactive compound formed by corrosion of Pu in liquid water or moisture at room temperature. The structural, electronic, mechanical, optical, thermodynamic properties of PuOH are studied by density-functional calculations within the framework of LDA/GGA and LDA/GGA+U. From the total energy calculation, we predict the lowest-energy crystal structure to have space group F-43m (No. 216). Within the LDA+U framework, the calculated lattice parameter of F-43m-PuOH is in good agreement with the experimental value and the corresponding ground state is predicted to be an antiferromagnetic charge-transfer insulator. Furthermore, we investigate the bonding character of PuOH by analyzing the electron structure and find that there is a stronger Pu-O bond and a weaker Pu-H bond. The mechanical properties including the elastic constants, elastic moduli and Debye's temperature, and the optical properties including the reflectivity and

absorption coefficient are also calculated. We then compute the phonon spectrum and verified the dynamical stability of F-43m-PuOH. Some thermodynamic quantities such as the specific heat are evaluated. Finally we calculate the formation energy of PuOH, and the reaction energies for the oxidation of PuOH and PuOH-coated Pu, which are in reasonable agreement with the experimental values.

*Keywords: PuOH, density functional theory, crystal structure*

## **Z-49**

### **Effects of Cr on the properties of WCoB ternary boride**

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Tungsten is a sort of scarce and unevenly distributed resources which have become a crucial issue all over the world. The way of developing an alternative materials with less or no tungsten in cemented carbides is a current research topic in the field of wear resistant hard materials. The wear resistant materials should have great physical properties in the industrial applications. Because of the intrinsic properties, boride can be used as a strong candidates in the field of wear resistant applications. However, the poor sinterability and brittleness of borides hinder the application in the process of manufacture. There is a new technology named reaction bronzing sintering which has been developed to form a ternary boride coexisting with a binder metal in the process of liquid phase sintering. The world first ternary boride base cermets have been made by this new technology with excellent mechanical properties, such as Mo<sub>2</sub>NiB<sub>2</sub>, Mo<sub>2</sub>FeB<sub>2</sub> and WCoB. This new technology can be used to save tungsten orcs by using less tungsten. The WCoB is a complex boride with extremely high hardness and excellent oxidation resistance. WCoB ternary boride base cermets are composed of a WCoB-type complex boride as a hard phase and a Co base matrix and contain less tungsten. The first principle by Castep in Material Studio can predict the properties and guide the way of experiment to check the result by the first principle. The radius of chromium atoms is similar to the radius of cobalt, which indicates it can replace the position of cobalt in the lattice. So chromium is used to replace cobalt and the properties can be predicted by simulation. The simulation shows the existence of replacement and the bond parameter. By using the data in simulation, the mechanical properties can be calculated and compared with the data in experiment. By using the elemental powder and pipe furnace, the manufacture and test of samples comply with national standards. The experiment shows that 15mass% Cr addition leads to the structural change of the Co from hexagonal close-packed to face-centered cubic and results remarkable mechanical properties change and structural refinement of the cermet in WCoB ternary borides base cermets. 20mass% Cr addition causes the appearance of new substance Co<sub>7</sub>W<sub>6</sub> and the reduction of mechanical properties. In summary, the elastic constants, mechanical anisotropy and electronic of WCoB were calculated by first principles calculations based on the density functional theory. The cohesive energy and formation enthalpy show that these compounds are thermodynamically stable. The elastic constants of these compounds are estimated using stress-strain method and the results satisfy all of the mechanical stability criteria. The Voigt-Reuss-Hill approximation is used to calculate the bulk moduli, shear moduli, Youngs moduli and the results shows similar results with the experiments data. The mechanical and physical properties of the hard phase of WCoB ternary boride base cermet were examined by using 5,10,15,20 mass% of Cr added WCoB ternary boride. Crystal structure of Co changes from HCP to FCC around 10 mass% Cr with the orthorhombic structure of WCoB ternary

borides. Cr added WCoB ternary borides, especially 15 mass% Cr shows high hardness and high elastic modulus comparable to WC and TiC. Cr containing WCoB ternary boride is a suitable alternative material to replace wear resistant hard materials such as WC.

*Keywords: ternary boride, WCoB, physical properties*

## **Z-50**

### **Molecular dynamics study of the orientation effect in magnesium**

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Objective: To better understand the plastic deformation behaviors and mechanisms of magnesium and its alloys, experiments and atomistic simulations have been employed widely. However, for the molecular dynamic simulations, researches are mostly focused on the deformation behaviors along some specific loading orientations, especially along the c-axis or a-axis. The else orientation effects on deformation mechanisms in magnesium single crystals have been less studied. [Methods] Molecular dynamics simulation is used to study the tension and compression deformation of magnesium single crystals with different orientations. The angle between the loading axis and the basal direction ranges from 0° to 90°. [Results] The tension simulations exhibit the deformation mechanisms of twinning, slip, crystallographic reorientation and basal/prismatic transformation. For compression simulations, the basal, prismatic and pyramidal slips are responsible for the initial plasticity, and no twinning is observed. [Conclusions] The simulation results show that the initial defects usually nucleate at free surfaces, but the initial plastic deformation and the subsequent microstructural evolutions are various due to different loading directions. Here, under uniaxial [0001]-axis tension, basal/prismatic transformation with a rotation of 90° relative to the parent lattice is a popular and crucial deformation behavior. It also can accommodate the transverse and longitudinal deformations, simultaneously.

*Keywords: molecular dynamics simulations; magnesium; plastic deformation; orientation*

## **Z-51**

### **Materials Data Science, a Paradigm for Material Discovery and Innovation**

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Data science has been known as the forth paradigm for scientific discovery, besides experimentation, theory and calculation. Materials Genome Initiative (MGI), released in 2011, is a methodology to combine the computation, experiments and data together to accelerate the materials innovation with lower cost. MGI emphasizes that the digital data are one of the tools to materials innovation. Materials data collection and databases construction have long been carried out worldwide, and China has built two national materials databases, the Chinese materials scientific data-sharing network, and the China Gateway to corrosion and protection. However, MGI is pushing materials science towards the big data age with the characteristics of high throughput, massive, across scale and multiple dimensions, and the cloud computing is ever bigger challenge when exploring the value of the materials data. Data science, when combined with the materials science, is going to overcome the difficulties. The concept of Materials Data Science, whose three-tier architecture consists of materials data system, life cycle curation of materials data and material data mining & depth extraction, was put forward to shift the data into information and explore the knowledge of data driven materials innovation.

*Keywords: materials data, MGI, big data, data science, materials innovation*

## Z-52

### **Cooperative effect of silicon and other alloying elements on creep resistance of titanium alloys: insight from first-principles calculations**

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Creep resistance is one of the key properties of titanium (Ti) alloys for high temperature applications such as in aero engines and gas turbines. It has been widely recognized that moderate addition of Si, especially when added together with some other elements (X), e.g., Mo, significantly improves the creep resistance of Ti alloys. To provide some fundamental understandings on such a cooperative effect, the interactions between Si and X in both hexagonal close-packed alpha and body-centered cubic beta phases are systematically investigated by using a first-principles method. We show that the transition metal (TM) atoms with the number of d electrons ( $N_d$ ) from 3 to 7 are attractive to Si in alpha phase whereas those with  $N_d > 8$  and simple metal (SM) alloying atoms are repulsive to Si. All the alloying atoms repel Si in the beta phase except for the ones with fewer d electrons than Ti. The electronic structure origin underlying the Si-X interaction is discussed based on the calculated electronic density of states and Bader charge. Our calculations suggest that the beneficial X-Si cooperative effect on the creep resistance is attributable to the strong X-Si attraction.

*Keywords: titanium alloys, creep resistance, first-principles calculations*

## Z-53

### **The atomistic study on shape memory properties of Ni-Ti alloys**

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Molecular dynamics simulation were employed to investigate the shape memory properties of Ni-Ti alloy bulks. The effects of Ni composition ratio on phase transformation were studied. Heating and cooling processes were carried out to determine the phase transformation temperature and the equilibrated atomic structure. At low temperature, different loading conditions were applied to the bulk alloy till plastic deformation was observed. The atomic configurations before and after plasticity were inspected using both common neighbor parameter (CNP) and slip vector in order to identify twinning deformation or dislocation. Then, the plastically deformed bulk went through the heating cycle to examine whether it would restore to the original shape.

*Keywords: shape memory, martensite, austenite*

## Z-54

### **Investigation of the phase equilibria and micro-performance of the Ti-Ni-Hf system using diffusion triples**

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Ti-Ni-based shape memory alloys have been widely applied in fields of aerospace and biomedical due to their shape memory behavior, excellent biocompatibility and corrosion resistance. However, Ti-Ni binary shape memory alloys were mainly used in low-temperature applications because of low martensitic transformation temperature ( $<100^\circ\text{C}$ ). Advanced shape memory alloys with higher transformation temperatures need to be

developed. Hafnium addition was found to be beneficial in improving the martensitic transformation temperature of the Ti-Ni-based alloys; thus a better understanding of the phase equilibria in the Ti-Ni-Hf ternary system is very valuable for the design and development of novel Ti-Ni-Hf shape memory alloys for high-temperature applications. In the current study, phase equilibrium relations in the Ti-Ni-Hf ternary system were investigated using diffusion triples and several key equilibrated alloys. Based on the experimental results from electron-probe microscopy (EPMA) and X-ray diffraction (XRD), three isothermal sections at 923K, 1073K and 1173K were constructed for the first time. Meanwhile, the hardness and elasticity modulus of the Ti-Ni-Hf alloys as a function of composition were also obtained using nanoindentation.

*Keywords: Ti-Ni-Hf system, isothermal section, phase equilibria, nanoindentation*

## **Z-55**

### **Orientation-dependent Nanoscale Abrasive Wear of mono-crystalline silicon**

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As a fundamental substrate material of micro/nanoelectromechanical systems (MEMS/NEMS) and integrated circuit (IC), monocrystalline silicon has received much research attention during the last few decades. A great deal of efforts have been made in revealing its mechanical behavior and deformation mechanism at the nanoscale. It is unfortunate that the fundamental wear mechanism of silicon at the nanoscale is still far less clear.

Nanoscale abrasive wear is a key wear mode in Si-based MEMS containing sliding/rotating parts. In this paper, we perform a large-scale molecular dynamics simulation of two-body and three-body abrasive wear on the (100), (110) and (111) oriented mono-crystalline silicon surface. A new model for three-body abrasion proposed by the present authors in previous work is adopted in order to mimic the moving of the particle. In this model, a spherical diamond particle is placed between two mono-crystalline silicon substrates (first body). During simulation, the two first bodies relatively move with a constant velocity and a constant load is applied the normal direction. The Tersoff potential is used to mode the interactions between the silicon atoms because this potential gives the correct cohesive energies for the different phase, and the morse potential to the interactions between the silicon atoms and the diamond abrasion atoms. According to the nanoindentation experiments, five phases (Si-I,  $\beta$ -Si, Si-III, Si-XII and bct5 phase) have been identified. In order to identify these phases, the combination technology of modified coordination number (CN) considering the first and second nearest neighbors, radial distribution function (RDF) and bond angle distribution function (ADF) are applied. We focus on the orientation-dependent abrasive wear behavior and the phase transformation mechanism of monocrystalline silicon at the nanoscale. The results shows both the remarkable anisotropic abrasive wear behavior and structure phase transformation of monocrystalline silicon. Comparing with the (100) and (111) oriented silicon surface, the (110) oriented silicon surface has a shallow damaged layer, which shows the good wear resistance. This is very different from the orientation-dependent mechanical properties of mono-crystalline silicon, in which the mechanical behavior of the (110) and (111) oriented silicon surfaces are similar but quite different from the (100) oriented surface. The movement pattern of particle also has an important significant impact on the wear behavior. The nanoscale abrasive wear behavior is carefully linked to the phase transformation. Although the amorphous silicon is the final residual phase for three oriented silicon surfaces, the phase transformation route is very different. For the (100)

and (110) oriented silicon surface, the initial Si-I turns into the high density amorphous silicon beneath the moving abrasive particle and then transforms to a thick and slightly compact low density amorphous silicon which overlays the surface. But for (111) oriented silicon surface, the pressure-induced Si-II is observed beneath the moving abrasive particle and then also transforms to the low density amorphous silicon. No obvious distinction is observed in phase transformation between the two-body and three-body abrasion. Comparing the (100) and (111) oriented surface, massive bct5 phase in the abrasive wear of (100) and (111) oriented silicon surface can be found, which highlights the relationship between the forming of bct5 phase and the wear resistance.

*Keywords: three-body abrasion, two-body abrasion, silicon, molecular dynamics*

## **Z-56**

### **Structural and mechanical heterogeneities in metallic glasses**

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The atomic packing nature and its relationship with macroscopic properties in metallic glasses are a long-standing fundamental issue in condensed matter physics and materials science. In addition to extensive researches on local atomic structures, the structural heterogeneity has recently become the focus of research in metallic glass community because of its scientific importance in understanding glass formation and mechanical properties. In this talk, structural heterogeneity at the sub-nanometer scale will be revealed directly in the model Cu-Zr glasses. Moreover, mechanical heterogeneity at the nanometer scale will also be uncovered by modeling indentation experiments with molecular dynamics simulations. Further, the relationship between the structural/mechanical heterogeneity and the glass-forming ability and mechanical behaviors will be discussed. Our findings demonstrate that the alloy with less heterogeneity has better glass forming ability, and the mechanical heterogeneity is closely related to the structural heterogeneity during compression and tension deformation. Our findings will shed new insights into understanding of the structure-property relationship in metallic glasses, and might be also helpful for decoding the atomic structures of these glassy solids.

*Keywords: metallic Glass, structural heterogeneity, mechanical heterogeneity, glass forming ability, molecular Dynamics*

## **Z-57**

### **Formation mechanism and interface strength of superhard nanocomposites**

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By means of density functional theory and thermodynamic modeling, we unveiled the formation mechanism of nanocomposites through spinodal decomposition, and the superhardness via the calculations of stress-strain response during tensile and shear deformation. Taken Ti-Si-N as a prototype which consists of one monolayer SiN sandwiched between a few nm thick TiN layers, we underlined that the thin SiN layer may coherently form between TiN nanocrystals through spinodal decomposition. Although the bulk fcc-SiN is unstable, the TiN/1ML-SiN/TiN sandwich can be thermodynamic and dynamically stable. The weakest link in the TiN/1ML-SiN/TiN sandwich is found interestingly to be the bonds between Ti and N atoms within the interlayer next to the SiN<sub>x</sub> interface. It can be attributed to the ubiquitous Friedel oscillations that are found in electronically perturbed solids adjacent to the interfaces, where decohesion in tension and slip in shear occurs between the Ti-N

interplanar bonds next to that interface. The effect of interface thickness on the mechanical strength is further clarified. These results provide ways to design new, stronger and harder materials.

*Keywords: First principles calculation, spinodal decomposition, ideal strength, superhard nanocomposites*

## **Z-58**

### **Strengthening effects of single particles with different mechanical property in ultra-thin Rolling of AA1235 aluminum alloys**

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In aluminum foil rolling, the foil quality largely depends on the number and the size of pinholes in the foil. Pinholes are usually resulted from some secondary particles in the matrix of the foils. The secondary particles may lead to stress concentration at the boundary with the matrix, and are finally removed from the matrix by the accumulated particle-matrix boundary stress in the following rolling. Different types of particles would result in stress concentration at different levels. The three dimensional finite element modeling is used to simulate the strengthening effect of particles with different hardness in the matrix of AA1235 aluminum foils in foil rolling. It is found: while the hardness ratio of the second phase particle to the matrix is less than 4, stress concentration in the matrix near the secondary particle increases linearly with increasing the hardness of the secondary particle. While the hardness ratio of second phase particle to the matrix is more than 4, stress concentration in the matrix near the secondary particles increases slightly with increasing the hardness.

*Keywords: AA1235 aluminum alloy, single particle, strengthening effect, deform-3D*

## **Z-59**

### **Characterization of anisotropic mechanical behavior of AZ31 Mg alloy under non-proportional loading by means of crystal plasticity modeling**

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The anisotropic mechanical behavior of AZ31 Mg alloy was observed under non-proportional loading due to dislocation slip, twinning and de-twinning. In order to capture this anisotropy, crystal plasticity modeling with slip, twinning and de-twinning was employed. Consequently, the texture evolution and micro-scale deformation mechanism of AZ31 Mg alloy under tension-torsion non-proportional loading were studied. A polycrystalline model was built based on Representative Volume Element (RVE) method and deformation behavior under two different loading paths was discussed. The first one is pre-tension along the extruded direction followed by unloading and torsion. The second one is pre-tension and pre-torsion along the extruded direction and followed by unloading and torsion. It is found that the torsion yield strength corresponding to the first loading path is higher than simple torsion, however, the one corresponding to the second path is lower than the one for simple torsion. Meanwhile de-twinning is observed under the second loading path. The simulation results are agreement with experiments. It is believed that twinning nucleation is restricted by pre-tension, the fraction of twinning decreases under torsion after pre-tension which results in the higher yield strength during the first loading path. However, de-twinning is responsible for the lower yield strength in the second loading path, which is activated under lower stress than twinning.



*Keywords: AZ31 magnesium alloy, crystal plasticity, non-proportional loading, de-twinning*

## **Z-60**

### **Thermodynamic calculation of the liquidus surface projection of multi-component aluminum alloys**

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Most aluminum alloys used in industrial manufacturing are multi-component systems. Unfortunately, multi-component systems lack systematic research. The lack of research is especially evident for the liquidus surface projection of the multi-component system where most of the projections are currently drawn by hand. Based on the Al–Cu–Fe–Mg–Si thermodynamic database previously established by Yong Du's group, thermodynamic calculations were performed for the Al–Cu–Fe–Mg, Al–Cu–Fe–Si, Al–Cu–Mg–Si, Al–Fe–Mg–Si quaternary systems and the Al–Cu–Fe–Mg–Si quinary systems. The temperatures and compositions of the liquidus invariant reactions in the Al-rich corner for all of the above systems were calculated and compared with the experimental data. The liquidus surface projections in the Al-rich corner for Al–Cu–Fe–Mg, Al–Cu–Fe–Si, Al–Cu–Mg–Si and Al–Fe–Mg–Si quaternary systems were constructed. The calculated results are in good agreement with the literature data. Furthermore, the liquidus surface projections for the Al–Cu–Fe–Mg–Si quinary system in the Al–Cu, Al–Si and Al–Mg sides were presented. The current work provides a straightforward and accurate expression for the liquidus surface projections of multi-component systems. The expressions will facilitate the understanding of the multi-component alloy systems that are frequently used in industrial applications.

*Keywords: Al–Cu–Fe–Mg–Si system, liquidus surface projection, thermodynamic calculation, phase diagram*

## **Z-61**

### **An atomic-scale study of the Fe–Li solid/liquid interface properties**

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Stainless steels and liquid Li are the structure material and neutron generator, respectively, of the International Fusion Materials Irradiation Facility (IFMIF). The compatibility between stainless steels and liquid Li is a very important problem, which directly relates to the stability and lifetime of IFMIF. Acquiring the interface information is helpful to improve the compatibility between the constituent materials. The Fe–Li solid/liquid interface properties have been investigated carefully at different temperatures using molecular dynamics simulations and it is found that the interface properties show remarkable orientation dependences. The three low-index orientations of Fe substrate suffer different impacts from liquid Li on their relaxation behaviors. The fine-scale density profiles show that the liquid Li atoms near the Fe (001)/(110)-Li interfaces were dramatically layered along the interface normal under the influence from the Fe blocks. In these two cases, the two-dimensional density maps indicate that the first several layered Li atom layers present high degree of order as

the Fe (001) or (111) crystal plane, especially at relative low temperatures. For the Fe (111) case, only the first two atom layers (in the liquid side) near the interface show faintly visible symmetry of the Fe (111) crystal plane at 500K and present much lower degree of the lateral order than the ones in the other two interfaces. The coarse-density profiles show that the interfaces are not ideal planes but finite-width slabs, and the interface widths increase gradually as temperature increasing. It is also found that in these three cases the Li atoms near the interfaces diffuse faster than those in the bulk of liquid Li. More interestedly, the Li atoms near the Fe(111)-Li interface diffuse faster and invade into the Fe substrate easier than those near the other two interfaces. These orientation-dependent characteristics are well explained in terms of the different surface properties of the Fe substrates.

*Keywords: Fe-Li solid-liquid interface, molecular dynamics, diffusion property*

### **Z-62**

#### **Effect of WC/Co coherency phase boundaries on fracture toughness of the nanocrystalline cemented carbides**

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The effect of coherency WC/Co phase boundaries on the fracture toughness of the nanocrystalline WC-Co cemented carbides is studied by MD simulation method. The simulation results show that the nanocrystalline WC-Co cemented carbides with coherency WC/Co phase boundaries has higher fracture toughness than that without coherency WC/Co phase boundaries. Moreover, the mechanism of why coherency WC/Co phase boundaries can improve the fracture toughness of the nanocrystalline cemented carbides is also investigated. It is found the fact that the separation energy of the coherent WC/Co phase boundary is larger than that of the incoherent WC/Co phase boundaries is the main reason for this excellent mechanical property.

*Keywords: coherency phase boundary, fracture toughness, simulation*

### **Z-63**

#### **Diffusion kinetics of Ni-Co-based alloys and mobility databases**

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It is known that the diffusion process has much to do with not only the homogenization and solidification of metal castings, but also the forming and dissolving process of precipitated phase, high-temperature creep and various surface treatments. Diffusion simulations based on thermodynamic descriptions and diffusion mobilities permit prediction of various aspects of diffusion-controlled phenomena, such as diffusion coefficients, concentration profiles, microstructural stability and lattice plane displacement.

In the present work, the interdiffusion coefficients of ternary Ni-Co-based alloys were deduced from the concentration profiles of diffusion couples measured by EPMA (Electron Probe Micro-Analyzer). By means of the CALPHAD approach, the diffusion mobility of the fcc phase for Ni-Co-based alloys were assessed based on the experimentally determined interdiffusion coefficients and diffusion data from the literature. The development of a multi-component mobility database is in progress.

*Keywords: Ni-Co-based, diffusion, mobility, CALPHAD*

### **Z-64**

## **Ab initio investigation on engineering alloys**

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Accurate description of materials requires the most advanced techniques from both experimental and theoretical areas. In spite of numerous available techniques, however, the experimental study of the atomic-scale properties and phenomena even in simple solids is rather difficult. Conventional Iron-based alloys and multicomponent high-entropy alloys (HEAs) are among the most important engineering materials due to their excellent mechanical properties. In these systems, the above challenges become more complex due to the interplay between the structural, chemical, and magnetic effects. On the other hand, advanced computational methods based on density functional theory ensure a proper platform for studying the fundamental properties of materials from first-principles theory. To achieve excellent structural materials, it is vital to optimize alloy components and their ratios. Using the all-electron exact muffin-tin orbitals (EMTO) method in combination with the coherent potential approximation (CPA), we systematically study the single-crystal and polycrystalline elastic properties of Fe-based and HEAs alloys.

## **Z-65**

### **A front-tracking solidification model for simulation of microstructure evolution during multi-component alloy solidification**

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A front-tracking solidification model has been developed to simulate the dendritic structure evolution during multi-component alloy solidification. In the model the growth of dendrites is governed by heat and mass transport and a finite difference technique is employed to solve heat and solute diffusion during solidification. The model incorporates front-tracking technique to calculate and track the exact position of the Solid/Liquid (S/L) interface as a part of solution process and a new capture rule was designed and implemented in the model to efficiently track the growing S/L interface. The model has been evaluated and verified using simulated data from Al-Si-Cu alloy solidification. The simulated results reveal that solute redistribution, curvature of the S/L interface and anisotropy of interface tension are important factors in determining the dendritic morphology. The calculation of the S/L interface curvature and anisotropy of surface tension was found to be particularly important in determining the dendritic growth direction.

*Keywords: front-tracking model, dendritic growth, solidification simulation, multi-component alloy*

## **Z-66**

### **Dynamics of phase separation in Fe-Cr alloys with variational coarsening mechanisms**

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Phase separation of Cr-enriched  $\alpha'$  phase from non-classical nucleation and growth to spinodal decomposition in the Fe-Cr alloys were studied by the phase-field simulation, the dynamics of initial phase separation followed by the coagulate coalescence or Ostwald ripening were clarified. The initial phase separation is accelerated for the

increased composition and decreasing aging temperature. The separation of  $\alpha'$  phase by non-classical nucleation and growth presents four stages evolution, the coarsening is dominated by the Ostwald ripening mechanism with a small time exponent than that of the combined mechanism of coagulate coalescence and Ostwald ripening for the  $\alpha'$  phase separated by spinodal decomposition. The cube of average radius and time shows linear relationship at the coarsening stage, while the variation of coarsening rate constant is not completely consistent with the variation of time exponent obtained from  $\langle R \rangle \sim (t^*)^n$ . The results show that the dynamic exponent is related with phase separation and coarsening mechanisms which are determined by the composition and aging temperature of Fe-Cr alloys, the dynamics of phase separation are theoretically and practically significant for the thermal aging and microstructure prediction.

*Keywords: phase separation, dynamics, coarsening, Fe-Cr alloys, phase-field*

## **Z-67**

### **Mapping of possible Re-substitutional elements in Ni-based superalloys**

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Owing excellent high-temperature mechanical properties and high resistance to creep and fatigue at elevated temperatures, Ni-based superalloys are widely used in both aviation and land-based gas turbine environments. Due to their extensive application in extreme environments, their resistance to creep deformation must be as high as possible. One common strategy is to add the alloying elements with extremely low diffusion coefficients at high temperatures. Re exhibits fairly low diffusion coefficient in Ni alloys and can significantly improve the creep resistance of the Ni-based superalloys. Thus, Re has been added in both second and third generation of single crystal superalloys. However, more Re addition can induce harmful topologically packed phases (TCPs) and also increase the cost, which limit the usage of Re in the next-generation Ni-based superalloys. Therefore, great efforts have been made to find the suitable Re-substitutional elements of which diffusion coefficients are comparable with Re. Based on the pragmatic numerical inverse method recently developed in our group, high-throughput determination of the composition-dependent interdiffusivities of  $\gamma$  and  $\gamma'$  phases in Ni-Al-X (X = Rh, Ta, W, Re, Os and Ir) alloys at 1373~1573 K was performed in the present work. A comprehensive comparison among the interdiffusion coefficients in  $\gamma$  and  $\gamma'$  phases of Ni-Al-X (X = Rh, Ta, W, Re, Os and Ir) alloys at 1373-1573 K was then conducted in order to find out the possible substitutional element for Re in Ni-based superalloys. The comparison results indicate that fcc Ni-Al-Os alloys and fcc Ni-Al-Re alloys exhibit the lowest diffusion coefficients, followed by fcc Ni-Al-Ir alloys, while L1<sub>2</sub> Ni-Al-W alloys and L1<sub>2</sub> Ni-Al-Ta alloys exhibit the lowest diffusion coefficient. It is anticipated that the present results can serve as the important information for design of the next-generation Ni-based superalloys.

*Keywords: nickel based superalloys, re-substitutional elements, interdiffusion, numerical inverse method*

## **Z-68**

### **Study of laser-induced damage resistance of PVA film using numerical stimulation and experimental measurements**

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The laser-induced damage of fused silica at 355nm is the key limiter for improving power transfer efficiency in high power laser facilities, and for the lifetime of the optical components. The output surface of fused silica is

more fragile than the input surface due to the energy deposition and stronger impulse wave. We present here a general method for coating a polymer film on the output surface of fused silica to improve the LIDT by transferring the energy deposition and cushion the impulse wave. Poly ( vinyl alcohol) (PVA) is the ideal material to prepare a high LIDT film due to its high hydrophilic properties, good film forming, low UV adsorption and suitable reflective index. We prepared the PVA film by spin coating and measured its optical properties. The results showed that PVA film can improve the LIDT of fused silica ~20%. In the meanwhile, we used the method of Finite Difference Time Domain (FDTD) to numerical simulate the intensity distribution around the interface of fused silica and PVA film. The results revealed that PVA film can decrease the intensity of the output surface ~30%. It was concluded that coating a PVA film is an effective method to improve the laser-induced damage resistance of fused silica.

*Keywords: Laser-induced damage, PVA, FDTD*

### **Z-69**

#### **Effects of temperature on vibration-assisted nano-scratch of monocrystalline copper via molecular dynamics simulation**

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It has always been a debated issue to understand how the temperature has effect on machining mechanism of Vibration-assisted Machining (VAM), particularly in atomic scale. In order to make it clear, a three-dimensional molecular dynamics (MD) modal of vibration-assisted nano-scratching on monocrystalline copper has been established. Embedded-Atom Method (EAM) potential is applied to describe interactions between copper atoms, and Morse potential is used for interaction of copper and carbon atoms. Surface quality of grooves, crystal defects and cutting force has been investigated in the simulations. Comparisons are made among the results of simulations from different temperature. According to the simulations, lower temperature leads to less crystal defects, and the groove quality of higher temperature is better. Higher temperature can also result in lower cutting force, including tangential force and normal force. The lower cutting force can decrease cutting energy, and can reduce tool wear. According to the analysis, VAM at higher temperature has positive effect on copper material machining.

*Keywords: molecular dynamics vibration-assisted temperature nano-scratching spherical tool*

### **Z-70**

#### **Simulating the plastic deformation of amorphous and crystalline solids at experimentally relevant timescales**

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he plastic deformation mechanisms, such as diffusion and dislocation motion and nucleation, dominate the plasticity of solids. However, they are usually infrequent events at ambient temperature which are far inaccessible to the normal molecular dynamics time window, and therefore exclude a direct atomic-scale observation of such

important mechanisms in solids. Here we conquer the timescale issues of simulating rare events in solids via state-of-the-art well-tempered metadynamics, and adaptive boost (AB) molecular dynamics. We demonstrate two categories of plastic events, one is diffusion in metallic glass, and the other is dislocation nucleation from grain boundary of crystal. In the former case, we find a transition from localized string-like diffusion to diffusion avalanche mechanisms in a model metallic glass with increasing temperature to caloric glass transition. In the latter case, we find a transition in the dislocation nucleation mechanisms from a shuffling assisted mechanism at experimental timescale to the nonshuffling mechanism at normal molecular dynamics timescale. These insights at wide timescales spanning many orders of magnitudes challenge our usual understanding of classic atomistic simulations of plastic deformations in solids.

*Keywords: metadynamics, adaptive boost, diffusion, dislocation, molecular dynamics*

## **Z-71**

### **A viewpoint of the yield criterion of amorphous alloy powders**

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Different from the structure of crystals with the long range order, the structure of amorphous alloy is short range order and long range disorder, which behaves with high strength, good corrosion resistance and wear resistance. As a yield model, Mohr-Coulomb model is adopted mostly in the finite element simulation of bulk metallic glasses, which gains many researchers' interests. But it is almost vacant in the field of amorphous alloy powders, the yield criterion of amorphous alloy powders obtained may provide theory base for fabricating bulk amorphous alloy by powder consolidation. In past two decades, a lot of preparation methods, such as copper mould suction casting, directional solidification, and powder consolidation, have developed to prepare bulk amorphous alloy. Among these preparation methods, powder consolidation covers yield and plastic deformation of amorphous alloy powders. As for yield behavior of amorphous alloy powders, finite element simulation has become one of the important means to study its forming process. Because of powder forming including volume shrinkage and particles deformation, it's necessary to establish a yield criterion of amorphous alloy powders based on the relative density and the hydrostatic stress. In addition, experimental datas are combined to verify the correctness of the FE-simulation. Yield criterion, together with flow rule and free volume model deduces elastoplastic model of amorphous alloy powder to accomplish FE-simulation of Powder consolidation.

*Keywords: amorphous alloy, powder consolidation, FE-simulation, yield criterion, hydrostatic stress*

## **Z-72**

### **Investigation of temperature effect on nanoindentation behavior of metallic glass via molecular dynamics simulation**

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The mechanical behavior of a binary  $\text{Cu}_{50}\text{Zr}_{50}$  metallic glass under various temperatures is studied through nanoindentation simulation via molecular dynamics. The effect of temperature from extreme low to high near glass-transition on the mechanical properties and deformation mechanics is focused. The load-displacement curves are obtained in various cases. Meanwhile, the atomic structure deformation, atomic stress, Von Mises shear

strain and temperature distribution are monitored throughout the simulation process. From the results, the glass in low temperature case has a higher hardness, a larger elastic range, a smaller average atomic displacement but a larger temperature rise. Furthermore, the results show that the glass under low temperature is prone to have a more inhomogeneous deformation and easier to form shear bands compared with higher temperature. The difference of icosahedral clusters in various cases is the key factor impacting the behavior of the glass. Low temperature glass has larger amounts of icosahedral clusters and thus more stable atomic structure, so that needs higher force to induce plastic deformation. Meanwhile, thermal uniformity makes it have less shear transformation activity, so that the glass tends to form inhomogeneous shear bands and has more local plastic deformation, thus causes larger temperature rising.

*Keywords: molecular dynamics metallic glass nanoindentation temperature effect*

### **Z-73**

#### **Degenerate seaweed to tilted dendrite transition in directional solidification: insights from phase-field simulations**

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We report the results of a phase-field study of degenerate seaweed to tilted dendrite transition and their growth dynamics during directional solidification of a binary alloy. Morphological selection maps in the planes of  $(G, V_p)$  and  $(\epsilon_4, V_p)$  show that lower pulling velocity, weaker anisotropic strength and higher thermal gradient can enhance the formation of the degenerate seaweed. The tip undercooling shows oscillations in seaweed growth, but it keeps at a constant value in dendritic growth. The M-S instability on the tips and the surface tension anisotropy of the solid-liquid interface are responsible for the formation of the degenerate seaweed. It is evidenced that the place where the interfacial instability occurs determines the morphological transition. The transient transition from degenerate seaweed to tilted dendrite shows that dendrites are dynamically preferred over seaweed. For the tilted dendritic arrays with a large tilted angle, primary spacing is investigated by comparing predicted results with the classical scaling power law, and the growth direction is found to be less sensitive to the pulling velocity and the primary spacing. Furthermore, the effect of the initial interface wavelength on the morphological transition is investigated to perform the history dependence of morphological selection.

*Keywords: directional solidification, seaweed growth, anisotropy*

### **Z-74**

#### **Modeling the massive-diffusive transition in multi-component substitutional alloys**

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Massive transformation (MT) has been extensively studied in the last century, which has been considered as interface-controlled and composition invariant. To compare with diffusive transformation (DT), which is controlled by the diffusion in bulk phases, MT is almost steady and several orders faster. The transition between MT and DT attracted many attentions in the past decades but completely different viewpoints about the critical limit between them were formed, which is considered to be the  $\alpha/\alpha+\gamma$  boundary, or the T0 line, in contrast. By using the combinatorial experiment approach, the critical limit is re-confirmed to be located in two-phase field. However, the controversy in the experimental results has not yet been solved by model.

The thermodynamic extreme principle (TEP) is a strong tool in the complex dissipation system, thus has been widely applied to the field such as phase transformation and grain growth. In the current work, TEP is applied to the austenite ( $\gamma$ ) $\rightarrow$ ferrite ( $\alpha$ ) transformation in multi-component substitutional alloys. The complex interfacial dissipate processes are considered in current as trans-interface diffusion and interface migration (i.e. interface friction). By this way, both MT and DT can be described by the current work.

Model is applied to Fe-Cr-Ni alloy firstly. The initial ferrite layer is assumed to be 2 nanometers. For a system of 2 $\mu$ m, MT can finish in several or dozens of seconds while DT is completed by several days. By adopting the uniform composition field as the initial condition, the critical limit between MT and DT is found to be located in two-phase field. However, when local equilibrium at interface is set as the initial condition, the critical limit is founded to moves to  $\alpha/\alpha+\gamma$  boundary. On the other hand, even the uniform composition field is adopted, the critical limit moves to  $\alpha/\alpha+\gamma$  boundary (or T0 line) when the mobility for trans-interface diffusion (or the mobility for interface migration) tends to infinite. At last, model is used to the Fe-Ni alloy, by adopting the appropriate trans-interface diffusion parameter, the experimental results by composition gradient technique is predicted.

In summary, the current model is applicable to the diffusion-controlled in multi-component alloys. Both the modes of MT and DT can be described well, with the appropriate trans-interface parameters, the experiment results can be predicted by current model. The calculation results are applicable to explain the significantly different conclusions for the transition between MT and DT from experiment results even in the same alloy system but different experiment approach.

*Keywords: massive transformation, phase transformation, diffusion, kinetics, thermodynamic*

## **Z-75**

### **The numerical simulation of hot die forging process of Ti-6Al-4V alloy blade**

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Ti-6Al-4V alloy is used extensively in aerospace applications due to its excellent properties. In this paper, the hot die forging process of the Ti-6Al-4V alloy blade was simulated by using 3D finite element method. Based on the model, the effect of process parameters on the deformation was investigated. Results show that the increase of temperature is beneficial to improving the uniformity of stress distribution and reducing the strain gradient. The slower the declining velocity of upper die, the smaller the strain gradient of severe deformation area. In addition, stress distribution gets uniform with velocity decreasing. The small friction coefficient can make strain distribution uneven and cause symmetry of stress distribution. The proposed numerical simulation of hot die forging of blade in the present work may yield important information for the development of hot die forging techniques and the manufacture of blade.

*Keywords: Ti-6Al-4V alloy, hot die forging, process parameters, numerical simulation*

## **Z-76**

### **Ab initio calculations of second-, third-, and fourth-order partial and inner elastic constants of diamond**

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By means of ab initio calculations, a unified framework is presented to investigate the effect of internal displacement on the linear and nonlinear elasticity of diamond crystal. The calculated anharmonic elastic constants, internal strain tensor and internal displacement in single diamond crystal are fully compatible with the available experimental data and other theoretical calculations. The complete set of second-, third- and fourth-order elastic constants and internal strain tensor are given, offering a better insight into the anharmonic and anisotropic elasticity behaviors and filling the gap of fourth-order elastic constant of diamond. This study provides a route for calculating the effect of internal strain on the elastic constants in a nonprimitive lattice. The pop-in event in energy-strain curve suggests that the number of elastic constant order required to depict the mechanical deformation of a material is determined by the deformation capability of a material.

*Keywords: ab initio, diamond, high-order elastic constants, internal displacement*

## Z-77

### The design of HEDM and novel electronic phenomena under high pressures

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High energy density materials (HEDM) have attracted more and more attention due to their wide potential applications as propellants and explosives. Among the family of HEDM, polymeric nitrogen has become a hot topic because its emission is nitrogen gas and is considered as a green and environmentally-friendly HEDM. In this field, the key issue is to searching for polymeric nitrogen that can stably exist in ambient conditions. Using CALYPSO technology companied by first-principles calculations, the high-pressure behaviors, including phase transition and electronic properties of pure nitrogen and alkali metal azides  $MN_3$  ( $M=Li, K, Rb, Cs$ ) have been studied. A cagelike nitrogen, named diamondoid N has been found. The diamondoid N adopts a highly symmetric body-centered cubic structure with 20 nitrogen atoms in a unit cell [1]. Our work reveals the phase transition and structural information of alkali metal azides under high pressures, and prove the polymerization of nitrogen in these compounds. The structural transition of  $N_3^-$  in azides is companied by hybridization type of nitrogen atoms from  $sp$ ,  $sp^2$  to partial  $sp^3$  induced by pressures [2, 6]. Under high pressure, post-transition metal Hg in Hg-F compounds transfers charge from the d orbitals to the F, thus behaving as a real transition metal [7, 8]. We demonstrate that Xe, Kr, and Ar can form thermodynamically stable compounds with Mg at high pressure ( $\geq 125$ ,  $\geq 250$ , and  $\geq 250$  GPa, respectively) [9]. The resulting compounds are metallic and the noble gas atoms are negatively charged, suggesting that chemical species with a completely filled shell can gain electrons, filling their outermost shell(s). Moreover, the calculations indicate that  $Mg_2NG$  ( $NG = Xe, Kr, Ar$ ) are high-pressure electrified with some of the electrons localized at interstitial sites enclosed by the surrounding atoms.

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*Keywords: high pressure, polymeric nitrogen, alkali metal azides, transition metal, high-pressure chemical activity*

## Z-78

### **Adsorbates induced work function change of metal and alloy surface: linking theoretical modeling to the electrochemical environment**

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Evaluating the potential of zero charge ( $E_{pzc}$ ) of metal–aqueous electrochemical interfaces has long been recognized as a key requirement for understanding the double-layer properties of these important systems. However, the experimental evaluation and even the meaning of  $E_{pzc}$  for metal–aqueous interfaces are complicated by the occurrence of potential-dependent chemisorption. As a consequence, it is very difficult, if not impossible, to evaluate the exact values of  $E_{pzc}$  by direct experimental measurement. Fortunately, the surface work function can be regarded as a bridge to link theoretical modeling to the electrochemical environment, since there is a common recognized linear relationship between the potential of zero charge and the work function in experiment. Therefore, the trend for  $E_{pzc}$  or its change  $\Delta E_{pzc}$  caused by adsorbates adsorption across different metal or alloy surfaces can be expressed, to a good approximation, in terms of  $\Phi$  or the corresponding  $\Delta\Phi$ . Here we adopt slab model calculations based on first-principles [1,2], and choose some simple charge-neutral species (C, H, N, O, S, OH, CH<sub>x</sub>, NH<sub>x</sub>, SH<sub>x</sub>) to investigate the adsorption induced work function change of the metal or overlayer bimetallic surface. Through our systematical and large-scale calculations, it would make an important step to understand the double layer properties in electrochemical systems.

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*Keywords: adsorbates, metal, bader-charge, work-function, dipole-moment, first-principle*

## Z-79

### **Investigation on change of NaCl properties in external electric field**

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NaCl is extensively applied in electro-plating, fuel cells and materials preparing. Further understanding properties of NaCl under external electric field has significant meaning. In this paper, first principles method is used to optimize the configuration of ground state of NaCl in electric fields vary from -0.030 to 0.03 a.u. The influence of external electric fields on the system energy, bond distance, charge distribution, band structure, density of states, thermal dynamic properties and Raman spectrum are studied. The results manifest that the molecular bond

distance and overall atomic charges gradually increase with the increase of the external electric field along the z axis direction. The charge distribution and fermi energy position have significant displacement compared with initial positions. Meanwhile, the system total energy, vibration frequency and Raman intensity decrease and the energy of dissociation becomes smaller with the increase of external electric field.

*Keywords: NaCl, electric field, first principles, fermi energy*

## **Z-80**

### **The two-step growth pathway to crystallization in a supercooled NiAl alloy**

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Crystallization of the supercooled alloys has the characteristic of non-equilibrium process. On this occasion, crystal growth mechanism has significant influence on atom arrangements, and further on material properties. However, despite its technological importance, the microscopic kinetics of crystallization is still elusive. A crucial topic about the mechanism of crystal growth concerns its kinetic pathways. To understand the structural evolution and the microscopic dynamics, we investigate the time-dependent crystallization behavior of the NiAl intermetallics using large-scale molecular dynamics simulations. The simulation results reveal that the crystallization process occurs via a two-step growth mechanism, involving the formation of initial non-equilibrium long range order (NLRO) regions and of the subsequent equilibrium long range order (ELRO) regions. Frequent merging and separating between large grains occurs through the gain and loss of the interfacial bridge atoms which belongs to NLRO regions. The instability of these NLRO atoms (atoms belonging to NLRO regions) directly reflects that the metastable NLRO atoms have the tendency to turn ordered. The newborn grains are rather inhomogeneous since the aggregated NLRO atoms distribute all around the grain. The subsequent rearrangement from the NLRO regions into the ELRO regions makes the grains more ordered and compact. The performance of the second step significantly impact the defect concentrations. The time evolution of the number of crystalline atoms in NLRO and ELRO regions demonstrates that a fraction of NLRO atoms will transform into ELRO regions. This confirms that the two-step growth mechanism should not be neglected. With respect to the structure, the evolution of the coordination polyhedra is actually the key controlling factor of this two-step growth mechanism. The transformation from five-fold symmetry to four-fold and six-fold symmetry along with the energy decreases guides the way of two-step growth. From liquids to NLRO and further to ELRO, the five-fold symmetry of these polyhedra gradually fades and eventually gives way to the crystalline B2 structure. Our simulation results may shed light on the underlying physics of the crystal growth process and present the rational foundation for further investigation of defect formation mechanisms.

*Keywords: crystallization, two-step growth mechanism, supercooled alloys*

## **Z-81**

### **Liquid/substrate interface in the heterogeneous nucleation during grain refinement of Al alloys**

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Grain refinement by inoculation is determined by heterogeneous nucleation and crystal growth. The physical process of heterogeneous nucleation on substrates, which depends on the nucleation potency of substrates, is still not fully understood. The present criterion for judging the capability of heterogeneous substrates only concerns the lattice misfit with nucleated crystal. To exactly understand the grain refining mechanism of  $\alpha$ -Al by the

Al-Ti-B master alloy, the  $\alpha$ -Al/solid-TiB<sub>2</sub> and liquid-Al/solid-TiB<sub>2</sub> interfaces were studied using the ab initio method. Different ordered structures were formed on the TiB<sub>2</sub> (0001) surface with different terminations, which determines the nucleation potency of TiB<sub>2</sub>. Five-layer quasi-solid region with a stacking sequence like fcc-Al (111) forms on the Ti-terminated TiB<sub>2</sub> surface, which is the basis of successful heterogeneous nucleation of  $\alpha$ -Al. The reason for using the Al-5Ti-1B master alloy as the commercial refiner in Al industries lies in two aspects: the excessive Ti atoms in the master alloy could guarantee the sufficient Ti chemical potential to form Ti-terminated surface of TiB<sub>2</sub>, and the locally stacking reconstruction induced by Ti atom relieves the accumulated elastic strain energy in ordered Al layers, facilitating fully heterogeneous nucleation on substrate. The simulation results were evidenced by the HRTEM and synchrotron XRD.

*Keywords: liquid-solid interface, heterogeneous nucleation, grain refinement, ab initio, molecular dynamics, solidification*

## **Z-82**

### **Rate theory model for the radiation-induced swelling in RAFM steels and implications for the radiation resistant design**

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As the advanced nuclear energy systems and fusion systems aim for safe, economic and clean energy resources. They raise higher requirements for the structural materials. The reduced activation ferritic/martensitic (RAFM) steel has been selected as the primary candidate structural material for the fusion DEMO and first fusion power plant, due to the good radiation resistance and low activation performance. The radiation-induced swelling (RIS) of RAFM steel will become significant under the high dose high energy neutron irradiation. In order to study the effects of alloy elements on the RIS in RAFM steels, a rate theory model considering the alloy-element-dependent diffusivity has been developed for various irradiation types, including electron, heavy-ion, and neutron irradiation conditions. The RIS has a minimum value around 9%Cr, which support that the radiation resistance of 9%Cr RAFM steel. The effects of other alloy elements can also be tested by using this model, and the research results will have potential applications for the optimization design for the radiation resistant RAFM steels and other similar materials.

*Keywords: rate theory model, radiation-induced swelling, RAFM steels*

## **Z-83**

### **A description of the formation of vacancy on grain boundaries in copper by structure unit model**

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Objective: It has been widely accepted that the grain boundaries (GBs) have a strong effect on the distribution of vacancy formed under irradiation. The degrees of the effect on the tendency of formation of vacancy on different GBs span a wide range. However, the regularity for the formation tendency and the mechanism for the effect are unclear. To address this issue, the tendency of formation of the vacancy on different GBs in Cu has been investigated, and then the mechanism is discussed. [Method] Molecular dynamics simulations of five Cu symmetric tilt grain boundaries were used to understand their interaction with vacancy. All calculations were performed using the LAMMPS program. The embedded-atom-method (EAM) potential developed by Mishin et al.

was chosen to describe interatomic interactions. [Results] The favorite site of the vacancy is affected by the detailed locations described by the structure unit model. The formation energy of vacancy at the common sites of neighboring structure units is higher than other sites. The vacancy has a same tendency of formation in the same structure unit irrespective of the grain boundary structure. The structure unit in grain boundaries results in the variation of the stress field in grain boundaries, and then the tendency of formation of the vacancy. The higher tensile stress, the easier vacancy form and the higher compressive stress the much difficult vacancy form. [Conclusion] The tendency of formation of vacancy on the GBs essentially depends on the variation of the stress field. The high compressive stress significantly increases the formation energy, while the high tensile stress decreases the formation energy. Because the variation of the stress field is coincident with the structure units, the tendency of formation of vacancy can be readily describe by structure unit model.

*Keywords: copper, vacancy cluster, grain boundary, atomistic simulation*

## **Z-84**

### **Simulation of hydrogen clustering behaviors on tungsten surface**

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Hydrogen (H) retention and blistering in tungsten (W) can significantly reduce the thermal conductivity and sputtering threshold of W, leading to a high content of tungsten impurity, resulting in the plasma extinguishing, and making the failure of the operation of fusion reaction. Therefore, H and H isotopes retention and blistering at tungsten surfaces under the plasma radiation is a key issue for the application of W-based plasma facing material. Thus, analyzing the dynamic processes of H retention, accumulation and blistering, revealing the mechanism of the formation of H-defect complexes, and controlling H blistering at W surfaces are crucial for W application. We employ a first-principles method and a molecular dynamics simulation using an embedded atom model (EAM) potential of W-H system developed by our group and compared with other interatomic potentials, to investigate the dynamic behaviors of H-defects and its clusters at W surfaces. The results show that hydrogen atoms are tend to cluster in the tungsten sub-surface based on the binding energy of hydrogen clusters calculated by both molecular dynamics and first-principles. Moreover, the binding energy of hydrogen clusters in the tungsten sub-surface is lower than that in bulk tungsten and is independent of the stress sign, which indicates that surface deformation and vacancy induced stress may be strongly conducive to the formation of hydrogen clusters. Our efforts would contribute to proposing a controlling method for the H blistering at W surfaces and could provide a theoretical reference for the application of W-based plasma facing material in the future tokamak fusion devices.

*Keywords: hydrogen, cluster, tungsten, surface, simulation*

## **Z-85**

### **Atomistic simulations of screw dislocations in bcc tungsten: from core structures and static properties to interaction with vacancies**

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It is generally recognized from both experimental and theoretical studies that the plasticity of bcc transition metals is controlled by the motion of  $1/2$  screw dislocations. Recent computational and experimental studies demonstrated that screw dislocations can increase hydrogen (H) retention in tungsten (W) by trapping H at the dislocation core [Terentyev D, et al. Nuclear Fusion, 2014, 54(4): 042004.]. However, the investigation of H bubble nucleation and growth necessitates the use of molecular dynamics based on interatomic potentials. An essential step towards revealing these dynamics is whether the core structures, static properties of dislocations and their interaction with defects from the interatomic potentials can reproduce the ab initio results. In this work, we use atomistic simulations to investigate the core structures, static properties of isolated  $1/2$  screw dislocations, and their interaction with vacancies based on three empirical interatomic potentials. Differential displacement maps show that only one embedded atom method potential is able to reproduce the compact non-degenerate core as evidenced by ab initio calculations. The obtained strain energy and stress distribution from atomistic simulations are, in general, consistent with elastic theory predictions. In particular, one component of the calculated shear stress, which is not present according to elastic theory, is non-negligible in the core region of our dislocation model. By calculating the binding energies between the dislocations and vacancies, we demonstrate that the dislocations act as vacancy sinks, which may be important for the nucleation and growth of hydrogen bubbles in W under irradiation.

*Keywords: screw dislocations, tungsten, vacancies, atomistic simulations*

## **Z-86**

### **Modeling the plastic deformation behavior of polycrystalline ferritic stainless steel using CPFEM**

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**Objective:** A 3D mesoscale model to characterize the plastic deformation behavior of ferritic stainless steel (FSS) was developed by combining a crystal plastic finite element model (CPFEM) with a cellular automaton (CA) algorithm. **[Method]** The polycrystalline geometry model was constructed using 3D CA firstly and then transferred to geometric mesh. The constitutive modeling of the plastic deformation of FSS was established by considering the  $\{110\}[111]$  and  $\{112\}[111]$  slip systems and applied to the finite element model by second development. The initial orientations of the grains were determined by selecting the actual orientations detected by EBSD. **[Results]** The results show that the developed CPFEM model is capable of modeling the stress-strain responses of polycrystalline FSS during deformation. The deformation behavior and the orientation transformation of the grains with different orientations were characterized by the developed model. The heterogeneity of local stress and strain distributions is captured. **[Conclusion]** The analysis indicates that the deformation behaviors of grains in polycrystal are not only related to the orientations but also to the interactions from adjacent grains.

*Keywords: crystal plastic finite element model, ferritic stainless steel, plastic deformation, cellular automaton*

## **Z-87**

### **A high-throughput approach to establish the atomic mobility database in multicomponent alloys**

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In this report, the concept of diffusion multiple and the idea for evaluation of atomic mobilities directly from the composition profiles was combined to serve as a high-throughput approach to establish the atomic mobility database in multicomponent alloys. By treating the simulation of composition profiles with the composition-dependent coefficients as the forward problem, the inverse coefficient problem that aims to compute the atomic mobilities directly from composition profiles can be postulated. The least square error method was employed to minimize the error between the simulated and the experimental composition profiles in order to solve the inverse coefficient problem. A comprehensive optimization strategy with the combination of the global grid minimization and the gradient free algorithm is implemented to find a feasible and satisfactory solution to the inverse problem. Finally, the presently proposed high-throughput approach was successfully applied to build the atomic mobility database of a fictitious quaternary system.

*Keywords: atomic mobility, diffusion, inverse coefficient problem, multicomponent alloys*

## **Poster**

### **Z-P01**

#### **First-principles study of lead iodide perovskite tetragonal and orthorhombic phases for photovoltaics**

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Methylammonium lead iodide perovskite,  $\text{CH}_3\text{NH}_3\text{PbI}_3$ , has attracted particular attention because of its fast increase in efficiency. Methylammonium lead iodide perovskite,  $\text{CH}_3\text{NH}_3\text{PbI}_3$ , has attracted particular attention because of its fast increase in efficiency as solid-state solar cells. We performed first-principles calculations with the nonlocal van der Waals (vdW) correlation to investigate the crystal structures and electronic and optical properties of  $\text{CH}_3\text{NH}_3\text{PbI}_3$ . The calculated results show that the distribution of methylammonium ions, which further changes the vdW interaction and hydrogen bonds of organic and inorganic matrixes, plays a vital role in both the geometry stability and the electronic structure. The vdW correlation is critical to provide appropriate descriptions of the interaction between the organic and the inorganic parts. The phase transformation from orthorhombic to tetragonal phase causes the decrease of the band gap and the red shift of the optical absorption coefficient.

*Keywords: DFT,  $\text{CH}_3\text{NH}_3\text{PbI}_3$*

### **Z-P02**

#### **Two-dimensional thermoelectric materials from high-throughput screening**

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Two dimensional (2D) materials have recently attracted much attention as their electronic structure and hence transport properties are different from their bulk counterparts. In this work, by high-throughput screening in the Inorganic Crystal Structure Database (ICSD), 92 layered compounds with Van der Waals interaction between layers were identified. By using density functional theory calculations, firstly the exfoliation energy of monolayer materials was calculated from geometry optimization, and then magnetic properties and band structures of both

bulk materials and 2D materials were calculated and compared. By comparing the magnetic properties, band edge states and band structures, the influence of dimension reduction on band structure and then thermoelectric properties was investigated. Results indicate that dimension reduction can change the band structure and tune the optical band gap, for example, MgPSe<sub>3</sub>, PbO and MX<sub>2</sub> (M=Mo、W; X=S、Se) have indirect band gap in bulk materials, while the indirect band gap changes to direct band gap after exfoliation into 2D monolayer. Change of the positions at band edges and shapes of band dispersion, as well as their influence on thermoelectric properties, were also discussed. Our work will help the design of new 2D thermoelectric materials.

*Keywords: two-dimensional materials, high-throughput screening, thermoelectric, first principles calculations*

### **Z-P03**

#### **Application of thermodynamic extremal principles to phase-field modeling of rapid solidification of multi-component alloys**

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The multi-component alloys play an important role in industry. But the studies about multi-component alloys are lacked. In this paper, a phase-field model for rapid solidification of a multi-component alloy system was developed based on the thermodynamic extremal principle. Thanks to the effective mobility approach (Acta Mater 2015;90:282), the model can introduces the non-equilibrium solute diffusion into not only long-range solute diffusion but the short-range solute redistribution. Property of the model under steady-state interface condition is analyzed and the simplified model is applied to planar solidification of Al-Si-Cu ternary alloys. A comparative study with the sharp interface model of Wang (Acta Mater 2013;61:1359) was performed and some advantages have been found. Abnormal partition behavior of certain alloys is happened due to the interaction effect between different components. The liquid solute profiles within the interface during solidification of Al-Si-Cu alloys were studied and further have a discussion about the definition of solute partition coefficient in phase-field methods. Contrary to the condition of equal diffusion potential in previous phase-field models (Phys Rev E 1999;60:7186), the diffusion potential jumps donot equal to zero in present model.

*Keywords: multi-component, rapid solidification, multi-phase-field model, Al-Si-Cu*

### **Z-P04**

#### **Experiment and simulation study of temperature field of jominy test of 7055 aluminum alloy**

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Temperature field research plays an important role in heat treatment. Jominy quenching test is the effective method of aluminum alloy heat treatment study including hardenability, quenching sensitivity of alloy and thermal stresses. In this paper, Jominy test of 7055 aluminum alloy with six different cooling conditions were set and the temperature fields were studied with simulation and experiment. The temperature fields was measured by sheathed thermocouples. Temperature at different distance through axis from quenching end and at radius direction of the same distance from end during the quench processing was recorded. The surface heat transfer coefficients of different cooling were calculated from the records. The heat conductivity and heat capacity of the material on different temperature were also got. The FEM (finite element method) modeling temperature field of quenching process was built using Marc software. The results of the simulation agree well with the experiments.



Above these tests, some parameters of 7055 aluminum alloy will pave the way for further research about material performance.

*Keywords: 7055aluminium alloy, jominy test, temperature field, finite element method*

## **Z-P05**

### **Texture grain growth of a 95% alumina ceramic in surface and multiphase-field study**

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The microstructure evolution of polycrystalline alumina during sintering has attracted much study consist of experimental and theoretical, but the grains in the surface have been paid little attention on. Firstly, this paper reported the texture grain growth of a 95% alumina ceramic (doped by silica and calcium oxide) in surface detected by the X-ray diffraction method, and the mechanism was discussed. In the 95% alumina ceramic, the grains with the basal plane parallel to the surface of the specimen grew preferentially, and the reason was conceivably that the surface made by the basal plane has a lower surface energy, which could be used to interpreted the plate-like grain growth during sintering of the calcium oxide doped alumina ceramic. Using 2D multiphase-field model, the surface energy being considered in the free energy density function, the texture grain growth of the 95% alumina ceramic in surface was simulated, and the simulation results were consistent with the experimental results qualitatively.

*Keywords: polycrystalline alumina, texture grain growth, multiphase-field*

## **Z-P06**

### **Micromagnetic simulation of a new L1<sub>0</sub>-FePt/X exchange coupled structure with low coercivity and high remanent magnetization**

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L1<sub>0</sub>-FePt with high uniaxial magnetocrystalline anisotropy constant ( $K_u$ ) has been currently considered as one of the promising materials to realize the ultrahigh density magnetic recording [1]. However, the coercivity of L1<sub>0</sub>-FePt exceeds the highest writing field that is supplied by current magnetic heads (about 20 kOe) [2]. An enclosed exchange-coupled structure was proposed to effectively decrease the coercivity of L1<sub>0</sub>-FePt for bit patterned media [3]. In this paper, a new structure based on the enclosed structure was proposed, which can reduce coercivity less than 20 kOe and maintain higher remanent magnetization. In addition, the new structure has better signal-to-noise ratios than the enclosed structure under the same stray field from the magnetic head.

The magnetic properties of two exchange coupled structures for bit patterned media were studied by the Object Oriented MicroMagnetic Framework software (OOMMF). Two exchange coupled structures based on cylinder shape are composed of soft and hard magnetic materials. The hard cylinder with diameter of 40 nm is surrounded by a 4-nm-thick soft part. For the enclosed structure A, the hard cylinder with height as 20 nm is covered by the top soft phase. The new structure B is similar to the structure A. But the hard cylinder is divided into two parts and separated by soft phase. In this paper, the hard phase is L1<sub>0</sub>-FePt and the soft phase is Fe or Co.

The simulation results show that the coercivities of two type structures with different  $K_u$  ( $L1_0$ -FePt) are smaller than the highest writing field. The hysteresis loops are characteristic of uniform reversal, which means the soft phase is rigidly coupled to the hard phase. Compared with the structure A, the structure B can enhance the remanent magnetization when the two exchange coupled structures have the same soft and hard phase volume. In addition, the coercivity can be further reduced as the soft phase thickness increases. As the top soft phase thickness increases, the system is in exchange spring phase. For the structure B, a step appears in the hysteresis loop when the thickness of middle soft phase reaches 12 nm. In order to study the influence of a stray field from the magnetic head, the angular dependence of the switching field was simulated. For  $K_u$  ( $L1_0$ -FePt) =  $1 \times 10^6$  J/m<sup>3</sup>, the curve is roughly symmetric and similar to that of the single phase given by the Stoner-Wohlfarth model. For  $K_u$  ( $L1_0$ -FePt) =  $7 \times 10^6$  J/m<sup>3</sup>, the curve is more close to the Kondorsky model. For the same  $K_u$  ( $L1_0$ -FePt), the signal-to-noise ratios of the structure B is better than that of the structure A. In summary, the new structure can effectively reduce coercivity less than the highest writing field even for  $K_u$  ( $L1_0$ -FePt) =  $7 \times 10^6$  J/m<sup>3</sup>. Meanwhile, it can maintain higher remanent magnetization and better signal-to-noise ratios than the enclosed structure.

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*Keywords: micromagnetic simulation,  $L1_0$ -FePt, hysteresis loop, coercivity, switching field*

## Z-P07

### First-principles calculations on interfaces between Al and $AlB_2$ -type transition metal diborides

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It is well known that adding Al-Ti-B master alloy into aluminum is beneficial for grain refinement. A common consensus is that the  $TiB_2$  particles in the Al-Ti-B master alloy are effective heterogeneous nucleation substrates. In this paper, the interfaces between Al and the  $AlB_2$ -type transition metal diborides  $TMB_2$  (TM = Sc, Ti, V, Cr, Mn, Y, Zr, Nb, Mo, Hf and Ta) were studied by first-principles calculations, aiming to investigate the heterogeneous nucleation potential of  $\alpha$ -Al grains on  $TMB_2$  particles with same structure of  $TiB_2$ . It is demonstrated that the  $TMB_2(0001)$  surface models with more than seven to nine atomic layers exhibit bulk-like interior, while the interlayer relaxations localized within top three layers are well converged. The outmost atom type of  $TMB_2$  free surface mainly depends on the interfacial chemical potential. The variation of the interfacial energies between  $\alpha$ -Al and diborides were analyzed, showing the nucleant capacity of substrates is related to not only the lattice mismatch, but also the interfacial atomic interaction.

*Keywords: first-principles calculation, interface,  $AlB_2$ -type transition metal diborides, heterogeneous nucleation*

## Z-P08

### Characterization of anisotropy of AZ31 Mg alloy based on molecular dynamics

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Due to strong (0001) texture, different yield strength (SD effect) and hardening behavior were observed along rolling direction (RD) and transverse direction (TD) for AZ31 rolling sheet, which is named as anisotropy. In order to capture this anisotropic mechanical behavior, molecular dynamics was employed. Thus, the deformation mechanism of tension along different direction for AZ31 rolling sheet was studied at atomic scale and the origin of anisotropic behavior was discussed in the current work. It is found that basal  $\langle a \rangle$  slip was activated for tension along different directions without twinning. The distribution factor of basal  $\langle a \rangle$  slip is small due to strong basal (0001) texture; however, CRSS of basal  $\langle a \rangle$  slip is much lower than other slip systems, which results in basal  $\langle a \rangle$  slip activate during tension along different directions. The non-homogeneous distribution of c axis of initial texture for AZ31 rolling sheet along RD and TD leads to different contribution of basal slip to deformation, which results in the macro-scale anisotropic mechanical behavior.

*Keywords: AZ31 magnesium alloy sheet, anisotropy, molecular dynamics, basal slip*

## **Z-P09**

### **First principles study of the phase stability Pt-Ir-Y Intermetallics**

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By performed the first-principles method, the formation enthalpy and binding energy, electronic structure, elastic properties and structural stability of Pt-Ir-Y intermetallic compounds were investigated. It can be seen from the results of binding energy and the enthalpy of formation that  $\text{Ir}_2\text{Y}$  is the most stable compound and the order of phase stability is  $\text{IrY} > \text{Pt}_3\text{Y} > \text{Pt}_4\text{Y}_5 > \text{Pt}_2\text{Y} > \text{Ir}_2\text{Y}$  in the Pt-Ir-Y system. TDOS at the Fermi level ( $N(E_F)$ ) can reveal the stability and the lower of the TDOS the more stable of the intermetallic compound. As can be seen from the TDOS, the phase stability of Pt-Ir-Y intermetallic compounds is  $\text{IrY} > \text{Pt}_3\text{Y} > \text{Pt}_4\text{Y}_5 > \text{Pt}_2\text{Y} > \text{Ir}_2\text{Y}$ . Based on the calculated elastic constants, the bulk modulus B, shear modulus G, Young's modulus E and Poisson ratio  $\nu$  of five intermetallics in the Pt-Ir-Y system are obtained. It can be concluded from the results of elastic moduli that the order of B, G and E is  $\text{Ir}_2\text{Y} > \text{Pt}_2\text{Y} > \text{Pt}_3\text{Y} > \text{IrY} > \text{Pt}_4\text{Y}_5$ . According to values of Poisson ratio  $\nu$  and B/G, all of the intermetallic compounds in the Pt-Ir-Y system are ductile and  $\text{Pt}_4\text{Y}_5$  is the best ductile.

*Keywords: intermetallic compounds, binding energy, enthalpy of formation, density of states, elastic constants*

## **Z-P10**

### **Phase stability of Ti-Mo alloys with low Mo content**

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Metastability of  $\beta$ -type Ti alloys permits stress-induced transformations to occur, which can significantly influence their mechanical response. Four stress-induced transformations occur such as hcp  $\alpha'$  martensite phase, orthorhombic  $\alpha''$  martensite phase, hexagonal omega phase, and  $\{332\}$  deformation twins. Activity of these deformation mechanisms is a function of beta-phase stability as quantified by Mo equivalency generally lower than 20 wt.%. In recent years, using first principles to investigate the phase stability of Ti-Mo alloys has shown well performance; however, most of first principles calculations focus on their stability with high Mo content (stable beta-phase). Thus, it is significant to investigated the stability of beta-phase in Ti-Mo alloys with low Mo content (metastable beta-phase) by first principles. In present work, interaction between Mo and Ti,

formation energy and density of state (DOS) are investigated from first principles calculations to discuss the effect of Mo distribution and low Mo content on phase stability. The 54-atom supercell model of hypothetical beta-phase was composed of  $3 \times 3 \times 3$  alignment of bcc unit cell. The  $Ti_{1-x}Mo_x$  ( $x$  at.%/wt.% = 3.7/7.1, 5.6/10.5, 7.4/13.8, 9.3/17.0) structures was constructed by the method of supercell. The calculations were carried out using a first-principles with the projected augmented wave (PAW) method as implemented in the VASP (Vienna Ab initio simulation package) code. The exchange-correlation functional was treated within the Perdew-Burke-Ernzerhof (PBE) generalized gradient approximation (GGA). The results show that formation energy of Mo-Mo in next-nearest site ( $d_{Mo-Mo} = \sqrt{3}a$ ) is lower than that of Mo-Mo in nearest site ( $d_{Mo-Mo} = 0.5\sqrt{3}a$ ) by 2 eV. Therefore, one Mo atom is located in a next-nearest site of another Mo atom, and three Mo atoms distribute as triangle form with the same distance from each other. Moreover, addition of Mo to beta-Ti alloys decreases formation energy of beta-phase, indicating that beta-phase stability was enhanced. The lattice constants of beta-phase decrease with Mo addition. In addition, phase stability of Ti-Mo alloys with low Mo content is discussed in terms of calculated DOS.

*Keywords: metastable beta-phase, phase stability, low Mo content, first principles, formation energy*

## **Z-P11**

### **Theoretical design and computational screening of precursors for atomic layer deposition**

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An effective precursor is a prerequisite and key to the success of atomic layer deposition (ALD). Currently, the design of more effective precursors is an important aspect of the development of ALD technology. Theoretical design and computational screening methods for ALD precursors are discussed. Theoretical calculations can predict many properties of precursors, such as the bond strength between the metal and the ligand, the thermolysis energy and barrier, the chelation energy, the hydrolysis energy, the formation energy, and so on. Most of these calculated data are related to the stability and reactivity of the precursor, which can be used in the design and computational screening of new ALD precursors. In addition, precursor design and screening require consideration of the ALD reaction mechanism in order to predict the true reactivity of the precursor with the surface, namely the surface reactivity of the precursor, which reflects the essence of ALD technology. Such theoretical efforts are expected to provide guidance for the design of more effective precursors and thereby lead to an improvement of ALD applications.

*Keywords: atomic layer, deposition precursor, design computational, screening surface reactivity*

## **Z-P12**

### **Design of 2D organic materials for photocatalyst and magnetic storage device**

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Since the graphene boom, great efforts have been devoted to the two-dimensional (2D) materials with exciting perspectives of applications. Using first-principles calculations, we design 2D organic materials as photocatalyst with suitable electronic band structures and magnetic storage devices with large magnetic anisotropy. From a systematic study of the electronic band structures, work function, CBM/VBM positions, and optical absorption spectra, we identified the covalent triazine framework (CTF) as a new class of 2D visiblelight-driven

organocatalyst for water splitting [1]. Starting from CTF, we further design three series of covalent organic framework using bottom-up strategies, i.e., molecular selection, tunable linkage, and functionalization, and confirm their photocatalytic activity under visible light in terms of electronic band structures [2]. In addition, magnetic properties of 5d transition metal decorated 2D polyphthalocyanine framework (TM@Pc) have systematically investigated by means of first-principles calculations with inclusion of spin-orbit coupling [3]. Giant perpendicular magnetic anisotropy is found in W@Pc and Re@Pc. After decorating with a homonuclear transition metal atom, an overturn of easy axis is demonstrated and the magnetic anisotropy energy can be enlarged to over 30 meV for Os and Ir. Hence, these 2D materials can serve as promising candidates for future magnetic storage devices. Our theoretical predictions would ignite computational design of 2D organic materials of other technological applications.

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### **Z-P13**

#### **Ab initio Study of the Surface Energy and the Point Defect of $\beta$ -SiC**

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Silicon carbide (SiC) not only considered as a promising candidate fusion structural material, but also deemed as an important wide band-gap semiconductor materials. We have performed ab initio calculation of some microscopic mechanism of cubic silicon carbide (3C-SiC) based on density functional theory. The surface energies for 13 surfaces of 3C-SiC have been calculated and then the average surface energies compare with the experiment value. It is found that the (110) surface has the lowest surface energy. In addition, we systematic examined the formation energy and the diffusion barrier of the point defect (i.e. carbide vacancy, silicon vacancy, self-interstitial atoms, anti-site defect). The results shown that the carbide vacancy is lower than silicon vacancy.

### **Z-P14**

#### **Effects of interstitial nitrogen atoms on atomic oxygen adsorption on Fe (001) surface from ab initio calculations**

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Nitrogen alloyed in austenitic stainless steel can significantly improve the pitting corrosion resistance. The complex interaction of oxygen with metal surface is the core of metal passivation. However, the effects of the interstitial N atoms on the oxygen adsorption on fcc Fe surface are rarely reported. To address this issue, the adsorption energies and electronic structures are investigated to explain the effects of the interstitial N atoms. The DFT calculations were performed using a plane wave pseudo-potential code, Vienna ab initio simulation package (VASP), which implements the projector augmented wave method for the description of ion-electron interactions. The generalized gradient approximation (GGA) with the Perdew and Wang (PW91) functional for the exchange correlation interaction was used. For the pure Fe surface, the adsorption energies of the O atom at the hollow site are always lower than those at the top and bridge sites. The adsorption of the O atom on Fe surface with N atoms

is significantly decreased, comparing with pure Fe surface. The charge density difference shows that the Coulombic interaction dominates the adsorption of the O atom, and a large depletion of electron density of the surface Fe atoms oriented towards the O atom enhances the interaction. Moreover, the localization of the charge density difference at the O atom is obviously enhanced by an increase in the local nitrogen concentration. The hollow site is the most stable site for O atom adsorption. The adsorption is dominated by the Coulombic interactions between the O atom and the neighboring Fe atoms. The existence of the interstitial N atoms can enhance the adsorption ability by the increase in the positive charge of the Fe atoms through a charge transfer from the Fe atoms to the N atom.

*Keywords: ab initio calculation, Nitrogen, adsorption, Austenitic stainless steel*

## **Z-P15**

### **Effects of uniaxial strain on the structure evolution of vacancy clusters in FCC metals**

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It is well known that vacancies have tendency to aggregate into clusters, and these clusters often have certain structures. Further evolution of the clusters may form other types of defects, such as stacking faults and voids. All these defects generally have decisive influence on the performance of materials. On the other hand, the strain of structural materials under certain pressure plays crucial roles in the structures of vacancy clusters. However, the detailed effects and mechanism of the strain remains controversial because complex variation of the binding energies and structures of vacancy clusters as a function of strain have been explored. Therefore, the structure evolution of vacancy clusters under the uniaxial strain in Cu, Al, Ni, and Fe is systematically studied by computer simulation in this work, and a mechanism is proposed to explain the effects. Molecular statics simulation method and potentials based on embedded atom method (EAM) were used in this study. A FCC supercell of 16,384-atoms ( $16 \times 16 \times 16$ ) was established. For each cluster size, various arrangements of vacancies are examined to find the clusters with higher binding energy. The complex variation of the binding energy significantly depends on the type and orientation of the clusters. The binding energies of linear and close-packed planar (NCP) vary monotonously with the strain, while otherwise those of close-packed planar (CPP), tetrahedral-type, octahedral-type show a maximum at relatively low strain. Moreover, under tensile strain, the clusters tend to distribute along strain axis; under the compressive strain, clusters tend to distribute vertical to strain axis. Linear and planar clusters tend to align parallel (perpendicular) to the strain axis under tensile (compressive) strain. Moreover, both the {001} planar cluster and body cluster become the dominant types when the clusters grow under high strain. A mechanism that the local structure around a vacancy cluster tends to approach the ideal lattice structure without defects and strain has been applied to explain the effects of the uniaxial strain on the relative stability of the vacancy clusters.

*Keywords: atomistic simulation, vacancy, cluster, uniaxial strain*

## **Z-P16**

### **Stacking sequence dominated stability and strength of ultrahigh compressible tungsten carbides**

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Intrinsically hard and superhard materials have been widely investigated due to their extensive industrial applications. Tungsten carbide, as one of the most widespread traditional cemented carbide, can adopt structures with different lattice symmetries. In this work, we obtained several polymorphic tungsten carbides i.e. hP2[187], hP4[194], hP8[194], hP12[194], and cF8[225], (here the structure types are expressed by the Pearson symbols and space group numbers) with different stacking sequence through high-throughput first principles calculations, and explored the possibility to tune the strength of tungsten carbide by varying the stacking sequence of the lattice planes. Our results show that all above polymorphs except for hP12[194] are dynamically stable, and the metastable hP4[194]-WC has the highest plastic resistance, whereas hP2[187] structure possesses the highest elastic moduli. This work provides a way to design ultraincompressible and strong materials by varying the crystal lattice stacking sequence.

*Keywords: DFT, tungsten carbides, stacking sequence, mechanical strength*

### Z-P17

#### **Roles of surface functional group on mechanical strength of two-dimensional titanium carbide**

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MXene, as a new-developed promising two-dimensional (2D) material, has attracted increasing attention by virtue of its excellent properties. Compared to the well-known 2D materials, its superior conductivity and tunable mechanical property make it being potentially used in flexible conductive electronic device. By means of density functional theory, we show that the surface functional groups play important roles on stabilization and mechanical strength of MXene, with the oxygen functionalized one as the best. However, the precurrent long-wave phonon softening might restrict its intrinsic strength. Such strengthening can be attributed to the distinct charge transfers from the interior to the exterior with the introduction of functional groups. Our results provide a quantitative understanding of exploring MXenes potential applications in flexible electronic devices.

*Keywords: density functional theory, flexible device, mechanical strength, electronic structure, two-dimensional material.*

### Z-P18

#### **Investigation of precipitation kinetics in binary Fe–Cu and ternary Fe–Cu–Ni alloys via kMC method**

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**Abstract:** The precipitation kinetics of coherent Cu rich clusters in binary Fe–Cu and ternary Fe–Cu–Ni alloys during thermal ageing was modeled by kinetic Monte Carlo method (kMC). The kMC was driven by the vacancy mediated diffusion with a broken bond energy model. With the energy model parameterized by *ab-initio* data, the precipitation kinetics was analyzed by means of advancement factor and cluster mobility. The advancement factor of binary Fe–Cu is in good agreement with experimental results. The cluster mobility is revealed to be slower with Ni addition. This reduction effect of cluster mobility weakens with larger Cu cluster size. Because of the reduction

of cluster mobility, the precipitation appears to be slower in Fe–Cu–Ni than in Fe–Cu. The results provide an approach to understand the effect of solute elements on Cu precipitation kinetics in multi-component steels.

## **Published only**

### **The phase transformation of single crystal silicon at large indentation strain**

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We perform a large-scale molecular dynamics simulation of nanoindentation on the (100) surface of single crystal silicon at a large indentation strain and provide an unequivocal evidence for a transition in high pressure phases depending on indentation strain. At a low indentation strain (in the range of 0.069~0.146), the crystalline  $\beta$ -Si and bct5 phases are two only high pressure phases. When the indentation strain exceeds a critical value of 0.146, a crystal-to-amorphous transformation can be found. Accompanying with this amorphization, an distinct discontinuity in loading curve, known as “pop-in”, can be observed in the load-indentation strain curve. The structure characteristic and the further phase transformation in unloading of the high pressure amorphous phase are also discussed in this paper. The present results provide a new insight into the mechanical behavior and phase transformation of single crystal silicon in the nanoindentation.

*Keywords: Nanoindentation, single crystal silicon, molecular dynamics, phase transformation*

### **Modeling the precipitation kinetics of cementite in bainite in 0.17% carbon steel**

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Nanoscale cementite can be obtained in 0.17% carbon steel during isothermal treatment at 500 °C after ultra fast cooling (UFC) and thermo-mechanical treatment. The precipitation strengthening contribution to yield strength was more than 250 MPa, when the heat treatment time was less than 20 min. The carbon diffusion is impacted by Mn and Si, which are redistributed during the precipitation process. All the effects induced by substitutional elements can be manifested through the restricted carbon diffusion, which is equal to the carbon diffusion multiplied by adjustable parameters. Based on this, a kinetic model has been adapted to simulate the precipitation behavior of cementite involving the evolution of the number density per unit volume, radius of cementite over time, and the evolution of carbon concentration in matrix. An excellent agreement between the predictions of the model and experimental observations was obtained.

*Keywords: ultra fast cooling, nanoscale cementite, precipitation kinetics, precipitation strengthening, classical nucleation*

### **Prediction on mechanical properties of MoSi<sub>2</sub> with alloying elements (Cr, W and Nb) from the first principles**



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The mechanical properties of  $C11_b$   $MoSi_2$  with alloying elements (Cr, W and Nb) have been investigated using the plane-wave pseudopotential method of density functional theory. The elastic modulus, hardness and thermodynamic properties of  $MoSi_2$  with Mo substituted by Cr, W and Nb have been discussed using the calculated elastic constants. Compared to no-doping  $MoSi_2$ , the mechanical modulus of  $MoSi_2$  doping with Cr decrease drastically, and the Debye temperature of  $MoSi_2$  doping with W decreases clearly. However, the B/G ratio and Poisson ratio of  $MoSi_2$  doping with Nb increases obviously. These results indicates that  $MoSi_2$  doping with Nb have relatively good ductility and strong metallic characteristic. As shown in three dimensional contours of elastic modulus and these projections on the (001) and (010) planes, the anisotropy of Young's modulus and shear modulus is weak for  $MoSi_2$  doping with Cr and W, but is obvious relatively for  $MoSi_2$  doping with Nb. According to calculating the charge density and density of state, the electronic properties of  $C11_b$   $MoSi_2$  with different alloying elements have been presented to reveal the effect of alloying on mechanical properties. Our calculated results are in excellent agreement with the available experiments and other theoretical data.

*Keywords: MoSi<sub>2</sub>, alloying element, mechanical properties, first principles*

#### **Thermodynamic calculation of the rare earth permanent magnets: Fe-RE (RE=Ho, Er, Tm, Sm) binary systems**

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Nd-Fe-B permanent magnets with excellent comprehensive magnetic properties have been used in many industrial applications such as electric vehicle and wind power [1-2]. The Nd<sub>2</sub>Fe<sub>14</sub>B-based permanent magnets with heavy rare earth (RE) elements have much better temperature stability, higher energy product and coercivity [3]. In order to better understand the mechanism of the Nd-Fe-B permanent magnets with heavy rare earth elements, the investigation on the phase relations and phase diagrams of the RE-Fe-B ternary systems are necessary. As the key sub-binary systems in the RE-Fe-B ternary systems, the Fe-RE binary systems are studied firstly. In this work, the experimental data of phase equilibria and thermodynamic properties of the Fe-RE (RE=Ho, Er, Tm, Sm) binary systems in the published literature were reviewed firstly [3-7]. Based on available phase equilibria data and thermodynamic data, the Fe-RE binary systems were assessed thermodynamically using the CALPHAD method [8]. As a result, further experimental information and thermodynamic calculations would be required in order to develop thermodynamic database of the RE-Fe-B ternary systems, which is indispensable to study the relations between alloy composition, microstructure and magnetic properties of novel Nd-Fe-B-based permanent magnets.

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*Keywords: Fe-RE binary systems, thermodynamic calculation, CALPHAD, phase diagram*

### **Thermodynamic calculation of phase equilibria in the Mn-RE (RE=Nd, Gd, Dy) binary systems**

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The RE-T-X (RE=rare-earth, T=transition metal and X=Si, Ge, Sn etc.) ternary compounds have attracted much attention due to their interesting magnetic phenomena, including heavy fermion behavior, exotic-magnetism. Especially, the stable intermetallic compounds in the RE-Mn-Ge ternary systems have show complex magnetic behavior mainly due to the interesting interplay between the 3d and 4f magnetism and the strong dependence of the magnitude of the Mn moment and the magnetic state of the Mn sub-lattice on the Mn-Mn interatomic distances [1-2]. For example, REMnGe compound show spin glass behavior [3-4], while the REMn<sub>2</sub>Ge<sub>2</sub> compound also displays magnetocaloric effect [5]. As key sub-binary systems of the RE-Mn-Ge ternary systems, the information of phase equilibria and thermodynamic properties of the Mn-RE (RE=Nd, Gd, Dy) binary systems are indispensable to explore the RE-Mn-Ge alloys with better magnetic properties. In this work, the experimental data of phase equilibria and thermodynamic properties of the Mn-RE (RE=Nd, Gd, Dy) binary systems in the published literature were reviewed firstly. Based on the available experimental information, thermodynamic calculation the Mn-RE binary systems was performed using the CALPHAD method. As a result, further experimental investigation and thermodynamic assessments would be still necessary in order to develop thermodynamic database of the RE-Mn-Ge ternary systems.

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*Keywords: Mn-RE binary systems, thermodynamic calculation, CALPHAD, phase diagram*

### **Phase-field simulation of dendritic growth of AlCu alloy**

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In the paper, the KKS model for phase-field is used and The dendrite growth of a Al-2%Cu binary alloy were simulated by the model coupled with solute field and temperature field. The effects of solidification and the thickness of the interface on the growth of equiaxed dendrite, distribution of solute field and temperature field in undercooled liquid alloy were analyzed systematically. The result indicates that: the dendrite has well-developed secondary arms as kinetics coefficient increases. meanwhile, the segregation of the solute and the tip speed

increases, the tip radius decreases, and the solute segregation in solid-liquid interface increases. The result agrees well with Ivantsov theory .

*Keywords: phase-field model, Al-Cu dual single-phase alloy, dendrite growth, Ivantsov theory*

### **Research of oxygen reduction reaction on sulfur-doped graphene**

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Based on the pronounced catalytic activity of Sulfur-doped graphene in previous paper, this paper simulated oxygen reduction reaction (ORR) of S-graphene by first principle calculation. Two different models of sulfur-doped graphene sheets ( $C_{61}H_{19}S$  and  $C_{60}H_{18}S$ ) were built, keeping pyridine and pyrrole species, respectively. A DMol<sup>3</sup> molecular orbital package based on the density functional theory (DFT) was adopted to calculate the ORR process. All of these impurity graphene models were relaxed to arrive at its global minimum energy. During optimization and total energy calculation, electronic exchange-correlation energy functions represented in reciprocal space with the Perdew-Burke-Ernzerh (PBE) of functional type, which was based on a generalized gradient approximation (GGA) were used. Several parameters, such as geometry structure, reaction energy, and electronic structure, had been used to analyze and characterize the ORR ability of S-graphene with pyridine or pyrrole structure. During the ORR process, there exist four steps reactions. From the point view of geometry structure. In the first step of the reaction, the OOH molecule moves from original state to graphene and is absorbed to a carbon atom near sulphur atom. Then the sulphur atom moves out of S-graphene plane to bond with oxygen atom. The distance between sulphur and oxygen atoms (O1) reduce to 1.85 . After another H atom is absorbed on OOH in reaction 2, the distance between two oxygen atoms and O1 –graphene don't change any more, but the distance between the other oxygen atom and graphene reduces to 1.80 . When the ORR process occurs at reaction 3, the first H<sub>2</sub>O molecule is produced after another H atom joining. Then the distance between two oxygen atoms increase to 2.96 . And we find the distance of O2-graphene is also increase from 3.52 . So the first H<sub>2</sub>O is produced and escapes from S-graphene. Reaction 4 is same with reaction 3 although the graphene-OH is absorbed on different carbon atom near sulfur atom. So, evolution of geometry structure shows the OOH molecule is absorbed to a carbon atom near sulphur atom in S-graphene with pyridine structure, and can be decomposed into two OH molecules because of the distance between sulphur and oxygen atoms decreasing sharply in ORR process. However the OOH molecule is hardly absorbed on S-graphene with pyrrole structure because there doesn't exist any chemical bond between OOH molecule or decomposed product and S-graphene. From the point view of reaction energy. In the first step of the reaction, the reaction energy of OOH absorbed on S-graphene reduce to -0.1326eV with pyridine structure; but for the pyrrole structure its reaction energy decreases to -0.0502eV. When another H atom was introduced into the system, the reaction energies of S-graphene with pyridine structure are -0.7377eV, -1.4313eV, and -2.0575eV for the following reaction steps respectively. For pyrrole structure, its reaction energies are -0.6792eV, -1.9017eV, and -2.4523eV. Those results show that the reaction energies of OOH molecule absorbed on S-graphene and H<sub>2</sub>O produce are negative originated from their generated chemical bond. But the reaction energies of the ORR process for S-graphene with pyrrole structure are negative originated from its deformed structure. From the point view of electronic structure, we calculated the electron density and density of states. In the first step of the reaction, the HOMO and LUMO spatial distribution spread homogeneously in S-graphene with pyridine structure, After another H atom introduced in this system in reaction 2, the electrons standing long away from S atom in graphene

plane start to get together onto HOOH molecule. Scrutinizing the third and fourth steps of H<sub>2</sub>O produced reactions, their HOMO and LUMO are similar with each other and the same as that in first step of reaction. While in S-graphene with pyrrole structure, the LUMO spatial distribution is localized intensively in first step of ORR reaction, In the next three reaction steps, their HOMO and LUMO spatial distributions don't have any change. On the other hand, Compared with the total DOS of S-graphene-OOH with different structure, it is shown that they are homological with each other, but their PDOS has some difference in every ORR step. In the first step of the reaction, OOH molecule is absorbed on S-graphene in S-graphene with pyridine structure, the bonding peak at -0.85eV is exhibiting tall and upright, but its bonding peak split into two small branch peak at -9.5eV in S-graphene with pyrrole structure. At the second reaction step, there exist three bonding peaks for HOOH on S-graphene with pyridine structure in 0~-0.4eV. But for that on S-graphene with pyrrole structure, there exist a series disperse bonding peaks in 0~-0.4eV. In the following steps for both of them are identical with each other. So the OOH molecule absorbed on S-graphene with pyridine structure decomposed into OH and OH more easily than that on S-graphene with pyrrole structure. So, electronic structure shows that the OOH molecule easily bonded with S-graphene of pyridine structure comes from their unlocalized HOMO and LUMO spatial distribution. However, when the OOH molecule is absorbed on S-graphene pyrrole structure, the LUMO spatial distribution is localized intensively. The DOS exhibits their different catalytic activity originated from their different chemical interaction between OOH and S-graphene. The all results show that the OOH molecule is absorbed easily and decomposed into H<sub>2</sub>O spontaneously on S-graphene with pyridine structure. The catalytic activity of S-graphene with pyridine structure is originated from the strongly chemical reaction between the OOH molecule and S-graphene plane. But the same ORR process is hard to occur for S-graphene with pyrrole structure. So the poor catalytic activity of S-graphene with pyrrole structure comes from their only molecule force between OOH molecule and S-graphene. Thus, our findings open an avenue for detailed and comprehensive studies of catalytic activity for light elements doped on graphene.

*Keywords:* sulfur-doped graphene, oxygen reduction reaction, reaction barrier, density of states, spin density

### **Sensing mechanism of SnO<sub>2</sub> (110) surface to NO<sub>2</sub>: density functional theory calculations**

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It is necessary to development NO<sub>2</sub> gas sensors as NO<sub>2</sub> is a pollutant. While, different from the reducing gases, oxidizing gas NO<sub>2</sub> will put up a complicated sensing process. DFT calculations are necessary to perform to understand NO<sub>2</sub>-sensing mechanisms at the atomic level. We introduce NO<sub>2</sub> to SnO<sub>2</sub> (110) surface with oxygen species pre-adsorbed. The NO<sub>2</sub> sensing mechanism of SnO<sub>2</sub> surface strongly depends upon the concentration of oxygen in the ambient atmosphere. The direct interactions between NO<sub>2</sub> molecule and SnO<sub>2</sub> sub-reduced surface (with removed two fold-coordinated bridging oxygen rows) for very low oxygen concentrations shows that, NO<sub>2</sub> gas molecules interact directly with tin ionic sites instead of reacting with oxygen species, resulting an increase in resistance of SnO<sub>2</sub>. We investigate gas-sensing processes of interaction between NO<sub>2</sub> molecule and SnO<sub>2</sub> surface with pre-adsorbed oxygen species for the case of considerable high oxygen concentrations. Adsorbed molecular oxygen ions compete with adsorbing NO<sub>2</sub> molecules for available surface sites and electrons from the SnO<sub>2</sub>. As the availability of oxygen ions on the SnO<sub>2</sub> surface increasing, the interaction between NO<sub>2</sub> and adsorbed oxygen species give rise to a reducing interaction, which brings a decrease in resistance of SnO<sub>2</sub>.

*Keywords: gas sensing, NO<sub>2</sub>, oxide semiconductor, charge transfer*

### **Size-dependent melting temperatures of metallic nanorods**

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An analytic model for size-dependent melting temperature  $T_m(D,L)$  of metallic cylindrical nanorods has been proposed in terms of the unified nanothermodynamical model where  $D$  and  $L$  denote the diameter and the length of nanorods, respectively. As the model describes,  $T_m(D,L)$  decreases with decreasing  $D$  and  $L$  where the diameter effect is the principle factor while the length effect is the secondary one. Moreover, the melting temperature of nanowires is slightly larger than that of nanorods at the same diameter when no surface reconstructions take place during the melting process. The validity of the model is verified by the available experimental and MD simulations results of Sn and Ni nanorods.

*Keywords: melting temperature, size dependence, nanowires, nanorods, nanothermodynamics*

### **Elastic properties, phonon focusing and electronic structures of typical long-period superstructures Al<sub>5</sub>Ti<sub>2</sub> and Al<sub>11</sub>Ti<sub>5</sub>**

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Typical long-period superstructures (LPSs) Al<sub>5</sub>Ti<sub>2</sub> and Al<sub>11</sub>Ti<sub>5</sub> possess novel structure and have severe effects on the dislocation configuration, anomalous strengthening, operative deformation mode and mechanical properties. The microstructure, mechanical properties and phonon focusing of Al<sub>5</sub>Ti<sub>2</sub> and Al<sub>11</sub>Ti<sub>5</sub> LPSs are crucial for alloy design to meet specific requirements, so completely and precisely understood of these two LPSs in theory is necessary. In present work, first-principles calculations have been performed to systematically study the elastic properties, phonon focusing and electronic structures of Al<sub>5</sub>Ti<sub>2</sub> and Al<sub>11</sub>Ti<sub>5</sub>. The obtained lattice parameters are in good agreement with the experimental data. The elastic constants are calculated, and bulk modulus  $B$ , shear modulus  $G$ , Young's modulus  $E$  and Poisson's ratio  $\nu$  are further obtained. Both of the numerical indicators and the three dimensional images show that Al<sub>5</sub>Ti<sub>2</sub> and Al<sub>11</sub>Ti<sub>5</sub> are anisotropic and the anisotropy is slightly high for Al<sub>5</sub>Ti<sub>2</sub>. Three slowness surfaces are constructed for Al<sub>5</sub>Ti<sub>2</sub> and Al<sub>11</sub>Ti<sub>5</sub> to investigate the phonon focusing patterns, and the group velocity surfaces are also obtained to gain more insight into the elastic anisotropy. Due to elastic anisotropy, both of the slowness surfaces and the group velocity surfaces are nonspherical, and the anisotropy is highest for slow transverse mode, and then followed by fast transverse mode and longitudinal mode. The electronic density of states and charge density distribution of Al<sub>5</sub>Ti<sub>2</sub> and Al<sub>11</sub>Ti<sub>5</sub> indicate that due to strong hybridization between Al-2p and Ti-3d, there is a strong directional bonding between the Al and Ti atoms. Electronic structures reveal the underlying mechanism of elastic properties and phonon focusing for Al<sub>5</sub>Ti<sub>2</sub> and Al<sub>11</sub>Ti<sub>5</sub>. As structural alloys, the elastic properties and phonon focusing are the basic parameters for the technical applications. Therefore, the systematical investigation on the elastic properties and phonon focusing of Al<sub>5</sub>Ti<sub>2</sub> and Al<sub>11</sub>Ti<sub>5</sub> LPSs are very important. The electronic structures can further reveal the underlying mechanism.

*Keywords: elastic properties, phonon focusing, electronic structures, anisotropy, LPSs*