Mini-symposium B13
Accelerating the Discovery of Advanced Materials Using the Materials Genome Approach

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B13-01 Keynote
In Silico Search for Heterogeneous Catalysts
Thomas Bligaard
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Density functional theory (DFT) and kinetic rate modeling has reached a level of speed and accuracy where they can be used to describe rates of complete catalytic reactions on transition metal surfaces. The direct computational search for new catalytic materials is thereby within reach. However, the number of necessary DFT calculations to perform “design” currently makes such direct search prohibitively computationally demanding. To accelerate the design process, we derive a set of simple descriptors that can be effectively used to perform ‘‘design’’ on a level of speed and accuracy where they can be used to describe rates of complete catalytic reactions on transition metal surfaces. This allows us to construct a search space of significantly reduced dimensionality, thus enabling the fast computational screening for new catalyst materials. The methodology is applied to the search for new catalysts to be used for steam reforming and the methanation reaction. The methodology highlights the need for constructing large databases of reliably calculated materials properties. We further suggest a systematic methodology to estimate the uncertainties of scientific conclusions based on models that have been parameterized by DFT simulations.

B13-02 Invited
First Principles Study and Design of Functional Materials for Energy Applications
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Materials design using first-principles techniques is one of the ultimate goals in computational materials science. Recent advances in first-principles electronic structure theory and computing power has enabled us to perform knowledge-based computational design of materials with unique optical, electrical, magnetic, and thermal properties that are tuned to specific energy-related applications. This approach has now become a vital tool in accelerating scientific discovery of energy materials. In this talk, selective topics from my group’s recent studies will be discussed to illustrate how computational methods can be used to understand and design functional energy materials including earth-abundant PV absorber materials; materials for H2 production through PEC water splitting; transparent conducting materials; energy storage materials; and materials for solid state lighting.

B13-03 Invited
Computational Materials Design by Evolutionary Structure Prediction
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We have recently developed an evolutionary algorithms (EA) based method to enable the accurate and reliable prediction of structures from only a few information (such as chemical system, external conditions, etc). How does it work - and why? In this lecture, I will summarize its principles, and discuss the recent developments as follows.

1) Predicting structures containing complex molecular motifs. We designed a constrained EA to treat each motif as a building block with internal coordinates. This way significantly speeds up the structural search together with the evolutionary variation operators. It can be applied to study the crystal packing of a wide range of systems (including small molecules, pharmaceuticals, explosives, polymers and even inorganic complexes containing distinct molecular blocks).

2) Optimizing chemical compositional space. This function allows the automatic search for all the stable compounds with variation of chemical compositions, which can be used to study binary/ternary systems composed of both atomic and molecular blocks.

3) Predicting low dimensional system is different from predicting the bulk crystals. For instance, surface brings another independent thermodynamic parameter, chemical potential. Following this hint, we proposed an approach to automatically explore the phase diagram for multi-component system at the given thermodynamic conditions.

B13-04 Invited
Materials informatics modeling for the design of advanced materials
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Recognition and exploitation of patterns in chemical data lie at the heart of any systematic program for materials design, which goes by the name of the Materials Genome approach. We demonstrate here the synergistic combination of quantitative structure–property relationship (QSPR) modeling and first-principles ab initio (DFT and wavefunction based) computations for the design of materials with specific electronic and physical properties. Such synergy can leverage the power of first principles computations to supplement and guide experiments by helping to navigate chemical space and screen materials with the desired properties, providing high-throughput capability that is generally not available from ab initio computations alone. Applications considered include the design of polymers appropriate for high energy density capacitor dielectrics with a combination of high dielectric constant, good insulating characteristics and fast response, and the systematic investigation of nanoscale atomic clusters. Design and construction of descriptors for materials informatics, feature selection and model validation protocols, as well as best practices in statistical modeling will be discussed.

B13-05 Keynote
The Linking Data Driven Discoveries with ab initio approaches
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Main aim of the present talk is to couple data base driven discoveries with ab initio calculations. We will identify which type of structure is preferred over another for a given chemistry of compound, from which we can discover new classification schemes of structure/chemistry/property relationships that classical homologies do not detect. We will also extract and organize the underlying design
rules for the formation of a particular structure by quantitatively assessing the influence of each materials attribute. Hence we can discover new and yet to be predicted or experimentally discovered materials chemistries with novel properties. We will develop design rules to identify which sequence or combination of parameters defines properties leading to predictive scaling laws for chemistry-property relationships for these "virtual" materials.

B13-06 Invited

Materials Discovery via CALYPSO Methodology

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Materials design has been the subject of topical interests in materials and physical sciences for long. Atomistic structures of materials occupy a central and often critical role, when establishing a correspondence between materials performance and their basic compositions. Theoretical prediction of atomistic structures of materials with the only given information of chemical compositions becomes crucially important, but it is extremely difficult as it basically involves in classifying a huge number of energy minima on the lattice energy surface. To tackle the problems, we have developed an efficient CALYPSO (Crystal structural AnLYsis by Particle Swarm Optimization) approach [1-2] for structure prediction from “scratch” based on particle swarm optimization algorithm by taking the advantage of swarm intelligence and the spirit of structures smart learning. The method has been coded into CALYPSO software (http://www.calypsy.cn) which is free for academic use.

Currently, CALYPSO method is able to predict structures of three-dimensional crystals, isolated clusters or molecules [3], surface reconstructions [4], and two-dimensional layers [5]. The applications of CALYPSO into purposed materials design of layered materials [6], high-pressure superconductors [7], and superhard materials [8] were successfully made. Our design of superhard materials [8] introduced a useful scheme, where the hardness value has been employed as the fitness function. This strategy might also be applicable into design of materials with other desired functional properties (e.g., thermoelectric figure of merit, topological Z2 number, etc.). For such a structural design, a well-understood structure to property formulation is required, by which functional properties of materials can be easily acquired at given structures. An emergent application is seen on design of photocatalyst materials.


B13-07 Invited

Materials data in accelerating the process from materials design to mass production

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Data have become the fourth paradigm of scientific discovery, except theory, computation and experimentation. The Chinese national material database, that is, materials scientific data-sharing network, has been built since 2009. Experimentation of data of material fundamentals and the metallic, inorganic, organic, composites, biomaterials, energy, information, natural, construction and road materials, which are totally 610,000 data entries, are integrated and free accessible via http://matsec.ustb.edu.cn. Materials Genome Initiative (MGI), released by US President Obama in 2011, is a methodology to combine the computation, experiments and data together to accelerate the materials innovation with lower cost. Under the infrastructure of MGI, the material databases provide not only the raw data of materials fundamental, and performance properties, but the deep processing data, for novel materials discovery, performance promotion and data-driven materials design. The standards and specifications for materials data on data integration, curation, citation and policies and techniques for data sharing have to be settled urgently. Technique of map-reduce and data mining to deal with the distributed data sources and the stream data coming from the high-throughput calculation and characterization will be highly associated with the building of open materials databases in the near future.

B13-08 Invited

Design of Novel Magnetic Clusters from Genetic Algorithm

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We employed genetic algorithm (GA) incorporated with density functional theory (DFT) to search for the ground state structures of alloy clusters and to discover novel clusters with exciting magnetic properties. We find a ferrimagnetic VS112– cluster with bicapped hexagonal antiferromagnet-wheel-like structure and a total spin of 4 µB [1], which has been further confirmed by experimental anion photoelectron spectroscopy. The number of unpaired electrons in neutral and anionic VS112– clusters can be understood by the Wade-Mingsos rules for polyhedral clusters. In addition, our combined study of photoelectron spectroscopy and DFT calculations show that Fe2Ge1– and Cr2Ge1– (n=3–12) clusters exhibit robust ferromagnetic and antiferromagnetic behaviors, respectively, which are nearly irrelevant to the cluster size and geometry. Finally, we propose two onion-like icosahedral matryoshka clusters [2], i.e., Sn6Mn12@Sn20 and P063/Mn12@P082, which combine a large magnetic moment of 28 µB, a moderate HOMO-LUMO gap, and weak inter-cluster interaction energy, making them ideal building blocks in novel magnetic materials and devices.


B13-09 Invited

Study on the chemistry-structure-property relationship for new materials by a combined approach of artificial intelligence, physical based semi-empirical, first principles modeling and experiments

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It is a well-known challenge to derive chemical - structure - property relationships for new materials based only on the experiment and the first principles methods. On the other hand, data mining techniques progress well although they may not directly provide fundamental physics for the obtained relationship. We use a combined approach of experiment, first principles and physics based semi-empirical models aided by data mining techniques to develop these relationships for new apatite systems. In addition, electrical conduction limit of BiFeO3 is also predicted and tested experimentally, by using the same approach. Therefore, we demonstrate the power of materials genome techniques in the search of new ionic conducting and multiferroic materials which are crucial to alternative energy, biomedical and electronic applications.

1. Qiang Xu, Mushtaq Sobhan, Franklin Anariba, Jeffrey Weng Chye Ho, Zhong Chen and Ping Wu*, Transition metal-doped BiFeO3 nanofibers: forecasting the conductivity limit, Phys.Chem.Chem.Phys., 2014, 16, 23089
3. Yingzhi Zeng, Pei-Lin Mao, San Ping Jiang, Pearson Wu, Lan Zhang, Ping Wu*, Prediction of oxygen ion conduction from relative Coulomb electronic
interactions in oxyapatites, Journal of Power Sources 196 (2011) 4524–4532

**B13-10**

Ab initio design of perovskite-type materials for photovoltaics

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Currently perovskite materials of the type AMX₃ (A = Cs, CH₃NH₃; M = Sn, Pb; X = halogen) have been attracting great interest for photovoltaics application because of the reports of high conversion efficiency of about 15%. We have performed density functional theory (DFT) based electronic structure calculations using pseudopotentials and generalized gradient approximation (GGA) for the exchange-correlation functional, for a number of such materials to understand their improved performance and also to search for improved materials. Here we report results of our studies on the electronic properties of the tin-halide based inorganic perovskites CsSnX₃ (X = I, Cl, Br) and also the mixed halides CsSn(XₓYᵧ)₃. These materials have direct band gap and also the top of the valence band and the bottom of the conduction band have p character. Therefore these materials are expected to have p-p transition which is reported to be highly favorable for photovoltaic applications. Different doping configurations have been found to relax in either tetragonal or orthorhombic phases starting from a cubic structure. The calculated GGA band gaps for such distributions lie in the range of ~0.5 to 1 eV. By making a suitable combination of different halogens, we can modulate the band gap and therefore the photo-response of these materials.

**B13-11**

Designing rare-earth-free strong magnets from ab initio calculations

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Currently there is a need to discover strong rare-earth-free permanent magnets for device applications. Iron-alloys, Fe-(Co, Ni, Pt), are among the promising candidates and also important for magnetic recording as well as catalysis. At the nanoscale, magnetic materials often have significantly enhanced magnetic moments and developing soft-hard nano-composites is an important way to develop strong permanent magnets. In the search for Fe-based nano-alloys to obtain the highest magnetic moments, we have focused on Fe-Pt nano-alloys as FePt is a known hard magnet. Our studies on small Fe-Pt clusters with 2-10 atoms showed high magnetic moments (>3µB) on Fe atoms and enrichment of Pt at low coordination sites. Further studies on Fe-Pt nanoparticles of different sizes, compositions, and with different initial structures including bulk fragments, decahedral, and icosahedral show Pt segregation on surface and maximization of unlike bonds. This led us to design a 147-atom icosahedral Fe₁₇Pt₁₂ nanoparticle with almost equal composition of Fe and Pt, but there is a phase separation of Fe and Pt in the nanoparticle. The magnetic moments on Fe atoms below the surface lie in the range of 2.76-3.07 µB while the surface atoms have the value of 3.34-3.36 µB. Further results on superlattices will be discussed.

**B13-12**

High-throughput screening for novel high-k dielectrics through first-principles calculation

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As the scale of transistors is reduced to less than a few nanometers, the leakage current brings a serious problem to the device's reliability. To overcome the problem, high-k materials is introduced as the gate dielectrics to enhance the capacitance and block the leakage simultaneously. Both large permittivity and large band gap is required for ideal high-k dielectrics. Currently, HfO₂ is widely used as the high-k material, but a higher-k material is still desired to achieve further enhancement. To search new high-k materials, we conduct a high-throughput ab initio calculation for band gap and permittivity. Accurate and efficient high-throughput calculation is enabled by newly-developed automation code which consists series of delicate calculation methods in highly optimized manner. As a result, we calculated ~1,800 different structures of binary and ternary from ICSD and obtained total property map. From the property map, we confirm that the inverse correlation relationship between band gap and permittivity is roughly valid for most oxides. However, there are also many new candidate materials which show interesting material properties. Analyzing these materials, we discuss the origin of high k values and suggest two design rules to find unknown higher-k materials that can be identified in future.