



CSRC

第三届中国科学院计算材料学与计算化学论坛

会议手册

2017年12月13日-16日

中国·北京

第三届中国工程院计算材料学与计算化学论坛

尊敬的学者、专家和青年朋友们：

由中国工程物理研究院科学技术委员会主办的“第三届中国工程院计算材料学与计算化学论坛”，将于2017年12月13日-16日在北京计算科学研究中心举行。

近年来，随着分子模拟方法与计算机技术的飞速发展，各学科相互交叉渗透，模拟计算已成为与实验和理论并重的科学研究手段，在多个学科中正发挥着越来越重要的作用。计算科学与材料科学、化学相结合形成了计算材料学和计算化学，也是我院目前国防科学研究的重要手段之一。为提高我院计算材料与计算化学研究水平，2014年与2016年，我们相继举办了“中工程院计算材料学与计算化学首届论坛”与“第二届中国工程院计算材料学与计算化学论坛”，两届论坛均得到了院内外领导、专家和同仁的积极响应，会议取得了圆满成功。今年，在中工程院挑战计划项目进行之际，我们将举行“第三届中国工程院计算材料学与计算化学论坛”，特邀请全院相关领域的专家学者和青年朋友们参会！

热忱欢迎全院计算材料与计算化学领域的专家、学者和青年科技人员参加本次论坛，探讨交流，贡献新思路、新动态，分享新技术、新成果，以促进我院计算材料学和计算化学研究领域的蓬勃发展！

会议组织机构

主办单位：中国工程物理研究院科学技术委员会

承办单位：北京计算科学研究中心

会议主席：汪小琳 中国工程物理研究院科学技术委员会副主任

魏苏淮 北京计算科学研究中心材料与能源部主任

张朝阳 中国工程物理研究院化工材料研究所研究员

会议学术委员会：汪小琳 魏苏淮 高世武 黄兵 管鹏飞 张朝阳

祝文军 姬广富 王旭 万强 敖冰云 雷海乐

崔旭东 张平 陈军 肖永浩

会务联系人：冯 怡

北京计算科学研究中心

电话：010-56981722

邮箱：cmscc2017@csrc.ac.cn

特邀报告专家

姬广富	中国工程物理研究院流体物理研究所（一所）
张朝阳	中国工程物理研究院化工材料研究所（三所）
崔旭东	中国工程物理研究院化工材料研究所（三所）
杨增辉	中国工程物理研究院电子工程研究所（五所）
王建伟	中国工程物理研究院电子工程研究所（五所）
黄理	中国工程物理研究院材料研究所（七所）
卢海燕	中国工程物理研究院材料研究所（七所）
尹强	中国工程物理研究院激光聚变研究中心（八所）
孟令彪	中国工程物理研究院激光聚变研究中心（八所）
郑法伟	中国工程物理研究院应用物理与计算数学研究所（九所）
张蕾	中国工程物理研究院应用物理与计算数学研究所（九所）
肖永浩	中国工程物理研究院计算机应用研究所（十二所）
储祥蕃	中国工程物理研究院研究生院
王旭	中国工程物理研究院研究生院
黄兵	北京计算科学研究中心
管鹏飞	北京计算科学研究中心
张东波	北京计算科学研究中心
任志勇	北京计算科学研究中心
李隽	清华大学
孟胜	中国科学院物理研究所
刘利民	北京航空航天大学
尹万健	苏州大学

会议日程

报到注册

地点：北京计算科学研究中心 一楼大厅（领取会议资料）

时间：2017年12月13日 09:00-20:00

论坛议程

北京计算科学研究中心三层 第二会议室 | 2017年12月14日-16日

2017年12月14日 星期四	
08:00 – 08:30	签到
Morning Session I, Chair: 汪小琳	
08:30 – 08:45	<i>Welcome & Opening Ceremony</i>
08:45 – 09:00	<i>Photo Taking</i>
09:00 – 09:30 (30 minutes)	储祥蓄, 中物院研究生院 Effect of Nanodiamond surfaces on Drug Delivery Systems
09:30 – 10:00 (30 minutes)	李隽, 清华大学 单原子催化理论研究进展
10:00 – 10:15 (15 minutes)	余勇, 中物院四所 变形状态下高分子网链形成历史的数值模拟研究
10:15 – 10:35	<i>Tea & Coffee Break</i>
Morning Session II, Chair: 魏苏淮	
10:35 – 11:05 (30 minutes)	张朝阳, 中物院三所 Tale of TKX-50 and HA-based Energetic Ionic Salts—Structures and Responses to Thermal-Mechanical Stimuli
11:05 – 11:35 (30 minutes)	黄兵, 北京计算科学研究中心 Defect and Doping Properties in Functional Materials
11:35 – 11:50 (15 minutes)	黄丽, 南方科技大学 Searching for substrate-supported 2D topological materials
12:00 – 14:00	<i>Lunch (Canteen, B1 Floor) & Rest</i>
Afternoon Session I, Chair: 高世武	
14:00 – 14:30 (30 minutes)	孟胜, 中科院物理所 Quantum Engineering of Energy Conversion
14:30 – 15:00 (30 minutes)	张蕾, 中物院九所 共晶炸药微观电子结构-宏观晶体堆积-性能预测
15:00 – 15:30 (30 minutes)	张东波, 北京计算科学研究中心 第一性原理声子准粒子及研究实例铍的热力学相变
15:30 – 15:50	<i>Tea & Coffee Break</i>

Afternoon Session II, Chair: 张东波	
15:50 – 16:20 (30 minutes)	郑法伟, 中物院九所 材料中电子和声子结构的反折叠计算方法 and 应用
16:20 – 16:50 (30 minutes)	王建伟, 中物院五所 Theoretical investigations of vacancy diffusion in silicon
16:50 – 17:20 (30 minutes)	尹万健, 苏州大学 Perovskite Solar Cell: From Materials Properties to Stability Trend
17:20 – 17:35 (15 minutes)	邱睿智, 中物院七所 Stability of plutonium monoxide from first-principles calculation
17:35 – 17:50 (15 minutes)	谢朝阳, 中物院四所 基于元胞自动机的材料腐蚀演化模拟方法研究
18:00	<i>Dinner: Pickup to Sishitianyuan Restaurant</i>
2017 年 12 月 15 日 星期五	
08:30 – 09:00	签到
Morning Session I, Chair: 刘利民	
09:00 – 09:30 (30 minutes)	杨增辉, 中物院五所 基于系综密度泛函理论的材料激发态性质新算法
09:30 – 10:00 (30 minutes)	管鹏飞, CSRC 非晶态材料与物理的计算模拟研究
10:00 – 10:15 (15 minutes)	晏顺坪, 中物院四所 基于贝叶斯方法的轻材料潮解模型选择研究
10:15 – 10:35	<i>Tea & Coffee Break</i>
Morning Session II, Chair: 张朝阳	
10:35 – 11:05 (30 minutes)	姬广富, 中物院一所 A Review on Phase Transition of Energetic Materials
11:05 – 11:35 (30 minutes)	刘利民, 北京航空航天大学 The Nature of Excess Electrons and their Roles in the Photocatalytic Activity
11:35 – 11:50 (15 minutes)	胡淑贤, 北京计算科学研究中心 Computational Assessment of Crown Ether Complexes of Actinyls
11:50 – 12:05 (15 minutes)	黄河, 中物院七所 Phase stability of CrCoNi medium entropy alloy at finite temperatures
12:05 – 14:00	<i>Lunch (Canteen, B1 Floor) & Rest</i>
Afternoon Session I, Chair: 管鹏飞	
14:00 – 14:30 (30 minutes)	崔旭东, 中物院三所 Modified C-H ₂ potentials and its applications in the hydrogen storage with molecular simulations
14:30 – 15:00 (30 minutes)	黄理, 中物院七所 铜系材料中混价行为与价态涨落的第一原理计算研究
15:00 – 15:30 (30 minutes)	任志勇, 北京计算科学研究中心 Quantum mechanical modeling of nanoscale optoelectronic devices

15:30 – 15:50	Tea & Coffee Break
Afternoon Session II, Chair: 黄兵	
15:50 – 16:20 (30 minutes)	孟令彪, 中物院八所 二维 IIA/IIB 金属碳化物单层材料电子结构与力学特性
16:20 – 16:50 (30 minutes)	卢海燕, 中物院七所 Electronic structure of cerium based heavy-fermion materials by means of a first-principles many-body approach
16:50 – 17:20 (30 minutes)	肖永浩, 中物院十二所 高通量材料计算支撑平台 HSWAP 研发进展
17:20 – 17:35 (15 minutes)	周韦, 中物院二所 α -Zr 中辐照损伤初期大缺陷形成机制的分子动力学模拟
17:35	Dinner (Canteen, B1 Floor)
2017 年 12 月 16 日 星期六	
08:30 – 09:00	签到
Morning Session I, Chair: 任志勇	
09:00 – 09:30 (30 minutes)	王旭, 中物院研究生院 强激光场中的原子分子: 基本物理简介以及对数值计算提出的挑战
09:30 – 09:45 (15 minutes)	陈金繁, 中物院七所 钴酞化合物在乙腈-水混合溶剂中催化产氢反应的第一性原理研究
09:45 – 10:00 (15 minutes)	金光希, 中物院二所 强关联材料 $\text{La}_2\text{O}_3\text{Fe}_2\text{Se}_2$ 中的电荷与自旋涨落
10:00 – 10:20	Tea & Coffee Break
Morning Session II, Chair: 胡淑贤	
10:20 – 10:35 (30 minutes)	尹强, 中物院八所 Effect of water in Poly(vinyl formal): Insight from the Molecular Dynamic Simulation
10:35 – 10:50 (15 minutes)	周阳, 中物院三所 典型硝基芳香炸药的跨膜运输及其对膜的损伤
10:50 – 11:05 (15 minutes)	王晓媛, 中物院四所 MOF-5 材料力学与电学性质的第一原理计算
11:05 – 11:20 (15 minutes)	王鑫, 中物院七所 Phase stability of $\text{UT}_2\text{Al}_{20}$ (T=Mo, Nb, Ti, Zr) and electrinxwangonic structure
11:20 – 11:30	Closing Remarks
11:30	Lunch (Canteen, B1 Floor)

报告摘要

Effect of Nanodiamond surfaces on Drug Delivery Systems

Xiang-qiang Chu

Graduate School of CAEP, Department of Nuclear Science and Technology, Beijing, China

Nontoxic, biocompatible nanodiamonds (ND) have recently been implemented in rational, systematic design of optimal therapeutic use in nanomedicines. However, hydrophilicity of the ND surface strongly influences structure and dynamics of biomolecules that restrict in situ applications of ND. Therefore, fundamental understanding of the impact of hydrophilic ND surface on biomolecules at the molecular level is essential. In this work, the tRNA dynamics on ND surfaces are investigated by high-resolution quasi-elastic neutron scattering (QENS) spectroscopy and all atom molecular dynamics simulation techniques. To understand how the tRNA motion is affected by the presence of ND, the flexibility of the tRNA is analyzed by elastic neutron scattering and it shows a sharp increase around 230K in its hydrated form. The intermediate scattering function (ISF) representing the tRNA dynamics follows the logarithmic decay as proposed by the Mode Coupling theory (MCT). The dynamics of hydrated RNA on ND surfaces are compared with that of the freestanding hydrated tRNA molecules and dry tRNA on ND surfaces at the molecular level within the time range of picosecond to several nanoseconds. Both QENS experiments and MD simulations show faster dynamics of tRNA on ND surface compared to that of the dry tRNA on ND surfaces and freestanding RNA molecules. The strong, attractive interactions between ND, tRNA, and water give rise to unlike dynamical behavior and structural changes of tRNA in front of ND compared to without ND. Our new findings may provide new design principles for safer, improved drug delivery platforms.

References:

- [1] Dhindsa, G.K. *et al*, An ab Initio Investigation of Fluorobromo Carbene, *J. Phys. Chem. B* (2016), 120,10059

单原子催化理论研究进展

李隽

清华大学

以纳米催化为中心的多相催化是化学科学的重要领域之一。本报告将介绍近年来单原子及动态单原子催化理论研究的进展^[1-5]，并简要展望其发展趋势。

References:

- [1] B Qiao, A Wang, X Yang, LF Allard, Z Jiang, Y Cui, J Liu, J Li, T Zhang, "Single-Atom Catalysis of CO Oxidation Using Pt1/FeOx", Nature Chem. 2011, 3, 634-641.
- [2] X Yang, A Wang, B Qiao, J Li, J Liu, T Zhang, "Single-Atom Catalysts: A New Frontier in Heterogeneous Catalysis", Acc. Chem. Res. 2013, 46, 1740-1748.
- [3] YG Wang, D Mei, VA Glezakov, J Li, R Rousseau, "Dynamic Formation of Single-Atom Catalytic Active Sites on Ceria-Supported Gold Nanoparticles", Nature Commun. 2015, 6, 6511.
- [4] SR Zhang, L Nguyen, JX Liang, JJ Shan, JY Liu, AI Frenkel, A Patlolla, WX Huang, J Li, F Tao, "Catalysis on Singly Dispersed Bimetallic Sites", Nature Commun. 2015, 6, 7938
- [5] JC Liu, YG Wang, J. Li, "Toward Rational Design of Oxide-Supported Single Atom Catalysts: Atomic Dispersion of Gold on Ceria", J. Am. Chem. Soc. 2017, 139, 6190.

变形状态下高分子网链形成历史的数值模拟研究

余勇

中物院总体工程研究所

在热力学起伏原理基础上,本文采用虚拟等效变形方法描述了交联、断裂反应对理想分子网链末端距的影响,建立了变形状态下理想分子网链的形成模型,得到了构型熵自由能的演化方程。采用一维分子链模型,数值模拟了变形状态下分子网链的形成历史,即发生任意交联与断裂反应。模拟结果表明,断裂反应使分子链自由能呈现离散分布,而交联反应则使分子链自由能呈现连续分布。分子网链性质的非均匀性分布,有助于更深入理解高分子材料粘弹性变形行为和断裂行为。

Tale of TKX-50 and HA-based Energetic Ionic Salts——Structures and Responses to Thermal-Mechanical Stimuli

Chao-Yang Zhang

Institute of Chemical Materials, China Academy of Engineering Physics (CAEP)

Introduction of energetic ionic salts (EISs); High packing densities of HA-based EISs; Enhanced thermal stability of HA-based EISs in contrast to pure HA; Low thermal stability of HA-based EISs relative to others; And mechanism of TKX-50 against thermal-mechanical stimuli.

Defect and Doping Properties in Functional Materials

Bing Huang

Beijing Computational Science Research Center, 100193

It is well-known that doping and defects play a critical role for the use of semiconductors. In this talk we will discuss the role of doping and defects in transparent conducting oxides (TCOs) and halide double perovskites (HDPs) materials. 1) In TCOs, we show that TM doping in oxides can be classified into three categories (Type-I, II, or III) based on their TM d-orbital energy levels reference to the bottom of the conduction band of In_2O_3 . We also identify that Zr, Hf, and Ta (Type-III) are better potential donors than Mo and Sn in In_2O_3 for achieving higher carrier mobility and density. Our analysis and approach can also be used to improve the doping performance in other oxides. 2) In HDPs, we have determined the stable chemical potential region to grow HDPs without structural decomposition. Importantly, we find that the Ag-rich & Br-poor are revealed to be the ideal chemical potential conditions to grow n-type $\text{Cs}_2\text{AgInBr}_6$ with shallow defect levels. Moreover, we find that the conductivity of $\text{Cs}_2\text{AgInBr}_6$ can change from good n-type, poorer n-type to intrinsic semiconducting depending on the growth conditions.

Searching for substrate-supported 2D topological materials

Li Huang

Department of Physics, Southern University of Science and Technology, Shenzhen 518055

Using combined scanning tunneling microscopy (STM) measurements and first-principles electronic structure calculations, we extensively studied the atomic and electronic properties of $\sqrt{7}$ -InBi overlayer on Si(111). We propose and demonstrate an effective experimental process to successfully form a large well-ordered $\sqrt{7}$ surface by depositing Bi atoms on the In-Si(111)- 4×1 substrate. The STM images exhibit a honeycomb pattern. After performing an exhaustive computational search, we identified the atomic structures of the surface at In and Bi coverages of $6/7$ and $3/7$ monolayers, respectively. We discovered a new trimer model with a lower energy than the previously proposed model. The simulated STM images of trimer models confirm the presence of the honeycomb pattern in accord with our experimental STM images. Most importantly, we found that the surface is robust, preserving the topologically non-trivial phase. Our edge state calculations verify that InBi overlayer on Si(111) is indeed a two-dimensional (2D) topological insulator (TI). Moreover, hybrid functional calculations result in band gap up to 70 meV, which is high enough for room temperature experiments. Our findings lay the foundation for the materials realization of 2D-TIs by growing InBi overlayer on Si(111) substrate.

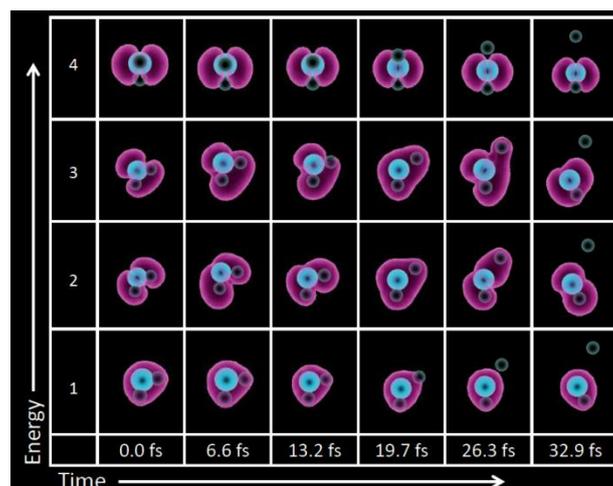
Quantum Engineering of Energy Conversion

Sheng Meng

Beijing National Laboratory for Condensed Matter Physics and Institute of Physics, CAS, Beijing 100190, China

It is argued that quantum pathways play a key role in energy conversion in natural processes such as photosynthesis. Here we study quantum couplings in artificial energy conversion systems including solar cells and photochemical synthesis. We first study light-induced interlayer ultrafast charge transfer in two-dimensional heterostructures. The charge separation process is generally hypothesized to be dependent on the interlayer stackings and interactions, however, the quantitative characteristics and detailed mechanism remain elusive. We demonstrate systematically the stacking-dependent interlayer charge transfer in MoS₂/WS₂ bilayer model system by first-principles time-dependent density-functional theory simulations. They show that the slight change in interlayer geometry can significantly modulate the charge transfer time from 100 fs to >1 ps scale. Detailed analysis further reveals that the transfer rate in MoS₂/WS₂ bilayers is governed by the electronic coupling between specific interlayer states, rather than interlayer binding strength, and follows a universal dependence on the specific-state-coupling strength. Surprisingly, this dependence breaks down the Fermi golden rule, as a result of strong interlayer coupling dependent coherent charge transfer.

Then ultrafast electron-nuclear dynamics of water splitting on gold nanoparticles upon exposure to femtosecond laser pulses was directly simulated using real time time-dependent density functional theory. Strong correlation between laser intensity, hot electron transfer, and reaction rates has been identified. The rate of water splitting is dependent not only on respective optical absorption strength, but also on the quantum oscillation mode of plasmonic excitation. Odd modes are more efficient than even modes, owing to larger amount of charge transfer and faster decaying into hot electrons whose energy matches well the anti-bonding orbital of water. This finding suggests photocatalytic activity can be manipulated by adjusting the energy level of plasmon-induced hot carriers, through altering the cluster size and laser parameter, to better overlap adsorbate unoccupied level in plasmon-assisted photochemistry.



References:

- 1) J. Zhang, H. Hong, C. Lian, W. Ma, X. Xu, X. Zhou, H. Fu, K.H. Liu, and **S. Meng**. Interlayer-State-Coupling Dependent Ultrafast Charge Transfer in MoS₂/WS₂ Bilayers. *Adv. Sci.* **4**, 1700086 (2017).
- 2) L. Yan, F.W. Wang, **S. Meng**. Quantum Mode Selectivity of Plasmon-Induced Water Splitting on Gold Nanoparticles. *ACS Nano* **10**, 5452 (2016).

共晶炸药微观电子结构-宏观晶体堆积、性能预测

张蕾¹、姜胜利¹、余一¹、赵艳红²、陈军^{1,2}

1. 中物院高性能数值模拟软件中心

2. 北京应用物理与计算数学研究所

共晶炸药的设计理念是从分子层面混合两种或多种高能炸药，并将分子按照一定的规则堆积排列，在保持炸药高能量密度的基础上改善其感度。基于我们自主研发的大规模并行第一性原理软件 HASEM，可以基于空间群、最密堆积准则和刚性分子堆积技术，对新型炸药分子进行全空间角搜索寻找全局势能最低点，预测炸药的晶体结构。基于实验标定的或理论预测的晶体结构，可基于 HASEM 软件揭示共晶炸药结构的热力学稳定机制，实现其力学、热力学、动力学和爆轰性能的预测，通过建立构效关系为新型合成的共晶炸药进行结构标定、性能和安全性预测。

第一性原理声子准粒子及研究实例铍的热力学相变

张东波

北京计算科学研究中心

声子概念是阐述固态材料热力学及热输运的重要理论基础。对于晶格非谐效应比较弱的体系，声子的模拟计算常用简谐近似或者准谐近似。但是，在非谐效应比较强的体系里面，这种计算方法不再适用。在声子的图像里面，晶格非谐可以理解为声子之间的多体散射作用。多数材料中，非谐在高温下普遍变得显著。基于第一性原理计算的声子准粒子方法，可以用来计算非谐声子谱与声子寿命，从而为高温高压材料热力学与热输运的计算研究奠定基础。以铍为例的热力学相变研究，充分体现了这个方法的使用条件与优点。

References:

- [1] Dong-Bo Zhang, Tao Sun, and Renata M. Wentzcovitch, Physical Review Letters 112, 058501 (2014)
- [2] Tao Sun, Dong-Bo Zhang, and Renata M. Wentzcovitch, Physical Review B 89, 094109 (2014)
- [3] Yong Lu, Tao Sun, Peihong Zhang, Ping Zhang, Dong-Bo Zhang*, and Renata M. Wentzcovitch, Physical Review Letters 118, 145702 (2017)

材料电子和声子结构中的反折叠方法及其应用

郑法伟

中物院应用物理与计算数学研究所

随着角分辨光电子能谱和中子非弹性散射谱等实验技术的迅速发展，电子能带和声子谱的实验测量变得越来越精确。然而对于结构复杂的材料，实验测到的电子能带和声子谱与理论计算的结果有本质的区别。反折叠方法是连接实验能谱与理论计算结果的桥梁，能够将理论计算的电子能带和声子谱进行反折叠处理，从而可以跟实验结果进行直接对比。在本次报告中，我将系统介绍反折叠方法的基本原理和应用，包括我们课题组近年来在这方面做的系列工作。

Theoretical investigations of vacancy diffusion in silicon

Jianwei Wang, Mo Li, and Jian Zhang

Microsystem & Terahertz Research Center, CEAP, China

The dynamical behavior of defects and impurities is one of central issues in fabricating semiconductor devices. The unintentional defects or impurities incorporated during the growth processes and designed doping affect the transport properties and then decide the performance of devices. The charge state shows a dramatically influences on the defect diffusion, and it has been labeled as charge enhanced diffusion and one example is recombination-enhanced diffusion. The pre-existing doping of other species also induces some influences on the migration of defects or impurities, for example, oxidation enhanced diffusions was discovered experimentally. The enhanced or retarded diffusions have been discovered experimentally for the charge states or the pre-existing doping of other species, but the completion of the two effects is still unclear, especially from an atomic view based on density functional theory calculations. Whether synergy effects of charge effect and doping effect can take place is investigated theoretically using diffusion behavior of vacancy in silicon as an example.

Perovskite Solar Cell: From Materials Properties to Stability Trend

Wan-Jian Yin

Soochow University

Perovskite solar cells based on prototype $\text{CH}_3\text{NH}_3\text{PbI}_3$ have recently shown remarkable performance. In this talk, I will present our theoretical research [1-7] in the last five years on those emerging class of solar cell materials. Firstly, I will give a brief introduction to the origin of superior properties of perovskite [1-5], including inverted band structure, high optical absorption, point defect tolerance and benign extend defect properties. After that, I will share our recent understanding on the perovskite stability [6,7], which is of the crucial importance in current perovskite field. We have found a new stability descriptor $(\mu+t)^\eta$, where μ , t and η are the octahedral factor, tolerance factor and the atomic packing fraction respectively, which performed much better than tolerance factor t that has been used for decades to judge the stability of perovskite. This thermodynamic stability trend may help efficient high-throughput searching of emerging stable perovskites and precise control of chemical compositions for stabilizing current perovskite.

References:

- [1] W.-J. Yin*, T. Shi and Y. Yan*, APL 104, 063903 (2014)
- [2] W.-J. Yin*, T. Shi and Y. Yan*, Adv. Mat. 26, 4653 (2014)
- [3] W.-J. Yin*, Y. Yan* and S.-H. Wei*, JPCL 5, 3625 (2015)
- [4] W.-J. Yin*, J.-H. Yang, J. Kang, Y. Yan and S.-H. Wei*, JMCA 3, 8926 (2015)
- [5] W.-J. Yin*, H. Chen, T. Shi, S.-H. Wei, Y. Yan*, Adv. Elec. Mater. 1500044 (2015)
- [6] Y. Yin, Y. Huang, Y. Wu, G. Chen, W.-J. Yin*, S.-H. Wei*, X.-G. Gong*, Chem. Mater. 29, 9429 (2017)
- [7] Q. Sun and W.-J. Yin*, JACS 139, 14905 (2017)

Stability of plutonium monoxide from first-principles calculation

Ruizhi Qiu, Xin Wang, Yongbin Zhang, and Bingyun Ao

Institute of Materials, CAEP

The resolution of questions about the existence of condensed plutonium monoxide (PuO) has long been hindered by lack of thermochemical data. Here we perform first-principles calculation to investigate the reaction $\text{Pu}_2\text{O}_3 + \text{Pu} \rightarrow 3 \text{PuO}$ and find that PuO is thermodynamically unstable under ambient pressure.

We also find PuO could be stabilized by pressure and impurities, such as carbon. The reaction $\text{Pu}_2\text{O}_3 + \text{Pu} \rightarrow 3 \text{PuO}$ becomes exothermal under pressure above 12 GPa. The origin of the stabilization under pressure lies in the delocalization of Pu-5f states and the increasing hybridization between Pu-5f/6d and O-2p states.

To illustrate the stabilization of PuO by carbon impurity, we performed first-principles calculations on the special quasirandom structures of plutonium monoxycarbide ($\text{PuO}_x\text{C}_{1-x}$) to investigate the physical property of monoxycarbide and its dependence on x . The solubility limit of oxygen is explored by examining the thermodynamical stability of plutonium monoxycarbide and monoxycarbide is found to be stable for $0 \leq x \leq 0.776$, which agrees well with the experiment. The stability of $\text{PuO}_x\text{C}_{1-x}$, or in other words, the stabilization of plutonium monoxide by carbon impurity, is ascribed to the established Pu 5f/6d-C 2p hybridization around the Fermi level. Moreover, the anomalous variation of experimental lattice parameter was also reproduced by our calculations. It was interpreted from the interplay between the increase of ionic radius and the shorter Pu-O bond with respect to Pu-C bond, rather than the reported intuitive mechanism of filling the vacancies and then replacing the carbon atoms.

基于元胞自动机的材料腐蚀演化模拟方法研究

谢朝阳

中物院总体所

核工业中核材料由于其化学活性强，极易遭受环境介质的化学、电化学作用而发生腐蚀，从而影响其物化性能和核性能。研究环境作用下的材料表面腐蚀损伤的形成和演化，对于定量描述结构材料的性能退化、评价结构的完整性、预测产品的剩余寿命具有重要的工程价值。金属材料在长期使用环境下会发生一定程度的表面腐蚀，如何认识腐蚀程度与时间和环境的关系是材料与结构性能退化以及寿命预测的关键环节。本文从计算模拟方法的角度研究表面腐蚀形貌变化，采用元胞自动机方法，对金属与气氛的化学腐蚀过程的元胞状态进行了分析，并定义了相应的演化规则，建立了 2 维情况下的材料表面腐蚀形貌变化模拟方法，以此为基础，分析讨论了不同参数环境条件下材料表面腐蚀形貌表征参数的变化规律，可为材料表面腐蚀形貌特征量的变化规律以及结构寿命预测等提供技术支撑。

基于系综密度泛函理论的材料激发态性质新算法

杨增辉

中国工程物理研究院微系统与太赫兹研究中心

半导体器件辐照损伤主要包括中子导致的位移损伤和 γ 射线导致的电离损伤。位移损伤过程中高速运动的初始碰撞原子对材料的电子态产生剧烈的扰动，电离损伤过程中 γ 射线导致电子激发，结果都是使材料的性质偏离材料在电子基态的性质。因此，对材料的电子激发态性质（如势能面、动力学过程、反应机理等）进行高效准确的计算对于研究辐照损伤是必需的。含时密度泛函理论(TDDFT)是目前最常用的电子激发态第一性原理方法，但由于计算量与体系大小的三次方成正比，只能对较小的体系（上百原子）进行计算，同时也有无法计算多电子跃迁、低估电荷转移激发态能量、难以正确描述束缚态激子等问题。我们基于系综密度泛函理论(EDFT)开发了全新的 Direct ensemble correction(DEC)算法^[1]，克服了 EDFT 传统方法的计算量远大于 TDDFT 的问题。DEC 算法的计算量与基态 DFT 基本持平，却能够在对原子体系激发能的计算中达到优于 TDDFT 的精确度（包括一般认为较难计算的 Rydberg states），且在不需任何特殊处理的情况下能够计算 TDDFT 目前无能为力的双电子激发态(double excitation)的能量。

References:

- [1] Z.-H. Yang, A. Pribram-Jones, K. Burke, and C. A. Ullrich, Phys. Rev. Lett. 119, 033003 (2017)

非晶态材料与物理的计算模拟研究

管鹏飞

北京计算科学研究中心

非晶合金，即金属玻璃，是一类特殊的由基本化学元素组成的非晶态物质，由于其独特的微观组织结构，展现出了不同于传统晶态合金材料的特殊物性，而成为高性能材料应用领域的重要一员。由于非晶合金的结构无序性，相应的理论模型也不完善，人们对非晶合金中一些基础物理问题的认识尚且不足，无法形成基本的理论框架来精确地描述其物性产生的微观机理。因而，当前非晶合金研究的核心问题可以概括为：如何建立以微观特征或结构为基础的基本理论框架，准确地概括非晶合金物性的微观机理。由于非晶合金微观结构的复杂性和实现精确实验表征的手段缺乏，计算模拟成为了研究非晶合金结构、物性及其关联的重要手段。基于计算模拟，我们通过对非晶合金体系的结构及其对外场的响应的系统研究，尝试理解非晶体系中的两个重要的物理过程：玻璃转变与剪切形变，并期望基于非晶合金中不均匀性的特征，理解和建立微观特征与物性之间的关联。本次报告我们将重点介绍非晶合金中短程有序结构与物性之间的退耦合关系，而中程序或更大尺度上的不均匀性可能将帮助我们更准确地理解非晶合金物性机理。

基于贝叶斯方法的轻材料潮解模型选择研究

晏顺坪

中物院总体所

LiH 是一种含氢量很高的材料, 在与水蒸气反应过程中能够释放出 95%~100% 的氢, 理想燃料比能达到 4900Wh/kg, 在聚合物电解质燃料电池领域具有广泛应用前景。尽管已有大量实验研究 LiH 材料在不同水分压条件下的反应动力学过程。本文在经典的化学反应速率方程中引入压力相关的系数, 提出几种压力相关的 LiH 潮解动力学模型, 并采用贝叶斯推论进行模型选择分析, 比较几种模型的优缺点, 给出最优的 LiH 潮解动力学模型。

A Review on Phase Transition of Energetic Materials

XU Wei-sen, JI Guang-Fu*

Institute of Fluid Physics, China Academy of Engineering Physics, Mianyang, China

This article reviewed the related research methods that usually used to study the phase transition of energetic materials. We introduced the commonly used experimental techniques of thermal analysis, ultrahigh pressure and impact loading, as well as many first-principle method and molecular dynamics theoretical simulation research methods with their application scope. The multiphase structures of nitramines, nitrides, nitrates, azoles and furazanes, as well as cage-like energetic materials under high temperature and pressure were summarized. The molecular configurations and crystal structures of the above energetic materials (including partially mixed explosives) in different phases are introduced. The phase transition characteristics and corresponding phase distributions of some materials under static and shock loading conditions are summarized. The phase transition mechanism revealed by high-precision theoretical simulation of some popular energetic materials is reviewed. Meanwhile, some results of phase transition point of energetic materials with several complicated phase transition mechanisms were found to be inconsistent. The crystal and molecular structure of some phases of PETN were inconsistent in different reports. The deep theoretical mechanism of large amount of phase transition is not revealed enough, and the microscopic mechanism of phase transition of mixed explosives is rarely involved.

The Nature of Excess Electrons and their Roles in the Photocatalytic Activity

Li-Min Liu

School of Physics, Beihang University

Recently, the defect effects on the advanced functional materials have been widely explored in my group[1-5]. In this talk, I will take TiO₂ as one example to show the intrinsic relationship between the excess electrons and the photoactivity. The defect TiO₂ is the vital topic of the semiconducting materials both because of the fundamental important of excess electrons and the widely applications. Transitions from the defect states are important for both the photoadsorption and photoactivity, however, the character of the electronic excited states is still unclear due to the great difficulty to experimentally characterize the unoccupied states. The detailed resonance states and its effects on the photoabsorption of defective TiO₂ are carefully explored with the first-principles calculations. The results show that the n-type defect TiO₂ exhibits two typical states, one is the gap state at ~1 eV below Fermi level E_F and the other at ~2.5 eV above E_F in the because of the Jahn-Teller effect, respectively. The calculated oscillation strength of the transition from the gap state to the corresponding resonance state at 2.5 eV further indicates the defect can enhance the photoabsorption.

References:

1. **Nature Energy** 2, 17111 (2017)
2. **Nature Comm.** DOI: 10.1038/s41467-017-01521-4 (2017)
3. **Nature Comm.** 7, 13638 (2016)
4. **Nature Comm.** 7, (2016)
5. **JACS**, 137, 9146 (2015)

Computational Assessment of Crown Ether Complexes of Actinyls

Shuxian Hu

Beijing Computational Science Research Center, Beijing

To further fundamental understanding of the nature and extent of covalency in actinyl–ligand bonding, and the benefits that this may have for the design of new ligands for nuclear waste separation, there is burgeoning interest in the nature of actinyl complexes with polydentate or multiple-point-donor ligands, such as crown ethers. There are few cases of structurally authenticated molecular actinyl–crown bonds under ambient conditions. We report here the computational characterization of AnO_{22+} –(15-crown-5) complexes, where $An = U, Np, Pu, Am,$ and Cm , and 15-crown-5 is the cyclic polyether ligand with five ether oxygen atoms. In the gas-phase complex the actinyl group is located inside of the crown ether, tilted slightly out of the plane of the five equatorial oxygen atoms that coordinate the actinide metal center. The actinyl–cyclic ether complexes are found to exhibit a conventional conformation, with typical An – O_{axial} and An – $O_{equatorial}$ distances and angles. A striking result is the enhanced stability of the insertion complex for UO_{22+} versus NpO_{22+} , PuO_{22+} , AmO_{22+} and CmO_{22+} , which is evaluated in the context of An – O binding strengths (esp. bonding covalency), and may have ramifications for the utility of actinyl–crown complexes in separations applications.

Phase stability of CrCoNi medium entropy alloy at finite temperatures

He Huang

Science and Technology on Surface Physics and Chemistry Laboratory, Mianyang 621900, PR China

The CrCoNi medium entropy alloy (MEA) has attracted much attention due to its exceptional mechanical properties at cryogenic temperatures. However, the phase transition in CrCoNi MEA is still a mysterious issue. The free energies at ground state and finite temperatures from 100 to 1200 K are calculated with exact muffin-tin orbitals (EMTO) method. The results show that fcc is the most stable phase at high temperatures and can transition to hcp structure below a critical temperature which is about 935 K thermodynamically. The reason for phase transition in CrCoNi MEA thermodynamically can be ascribed to the increasing different contribution of magnetic and vibrational entropy to free energies in fcc and hcp structure with the increment of temperatures. The trapping effect of atoms established by a seven bond interaction energy (SBIE) model probably inhibits the motion of atoms on the γ -surface kinetically and leads to unobserved phase transition of fcc to hcp in CrCoNi MEA at low temperatures and constant pressure experimentally.

References:

- [1] J.-W. Yeh, S.-K. Chen, S.-J. Lin, J.-Y. Gan, T.-S. Chin, T.-T. Shun, C.-H. Tsau, S.-Y. Chang, Nanostructured high-entropy alloys with multiple principal elements: novel alloy design concepts and outcomes, *Adv. Eng. Mater.* 6 (5) (2004) 299-303.
- [2] B. Cantor, I. Chang, P. Knight, A. Vincent, Microstructural development in equiatomic multicomponent alloys, *Mater. Sci. Eng. A* 375 (2004) 213-218.
- [3] J. W. Yeh, Y. L. Chen, S. J. Lin, S. K. Chen, High-entropy alloys-a new era of exploitation, in: *Materials Science Forum*, Vol. 560, Trans Tech Publ, 2007, pp. 1-9.
- [4] J.-W. Yeh, Alloy design strategies and future trends in high entropy alloys, *JOM* 65 (12) (2013) 1759-1771.
- [5] Z. Wu, Y. Gao, H. Bei, Thermal activation mechanisms and Labusch-type strengthening analysis for a family of high-entropy and equiatomic solid-solution alloys, *Acta Materialia* 120 (2016) 108-119.
- [6] G. Sathiaraj, M. Ahmed, P. Bhattacharjee, Microstructure and texture of heavily cold-rolled and annealed fcc equiatomic medium to high entropy alloys, *Journal of Alloys and Compounds* 664 (2016) 109-119.

Modified C-H₂ potentials and its applications in the hydrogen storage with molecular simulations

Xudong Cui

Sichuan New Materials Research Center, Institute of Chemical Materials, China Academy of Engineering Physics

In this talk, I will review some progress on the DFT theory, and hydrogen storage simulations with molecular dynamic simulations that have done in my group.

钢系材料中混价行为与价态涨落的第一原理计算研究

黄理

中国工程物理研究院材料研究所

在钢系材料中已经发现了许多反常的量子物理现象，其中它们的混价行为与价态涨落在近年来受到了比较多的关注。我们结合密度泛函理论以及动力学平均场方法，系统研究了若干个具有混价行为与价态涨落的钢系材料。本报告将选择一些典型的例子进行展示：(1) 立方相二氧化铀在压力的作用下将会发生具有轨道选择性的金属-绝缘体相变，系统的原子组态分布将会有巨大的变化。(2) 金属钷属于典型的混价体系，其六个同素异形体的原子组态分布有很大的不同。我们发现 $5f^5$ 组态的分布与原子体积存在着线性关系。(3) 金属铀的价态涨落非常显著，在压力的作用下，铀的价态将会在+3价与+2价之间变化。我们通过计算解释了其中的内部物理机制。

Quantum mechanical modeling of nanoscale optoelectronic devices

ChiYung Yam

Beijing Computational Science Research Center, Beijing, China

An efficient quantum mechanical approach is formulated to model electron-photon interactions in nanoscale devices. Based on nonequilibrium Green's function formalism, electron-photon interactions and open boundaries in the nanoscale systems are taken into account in terms of self-energies. By separating different components in the electron-photon interactions, optical absorption and emission processes in the devices can be analyzed, and the method allows studies of different optoelectronic devices. In conjunction with density-functional tight-binding method, photo-induced current and other optical properties of nanoscale devices can be simulated without relying on empirical parameters. To demonstrate our approach, numerical studies of nanoscale solar cells and light-emitting diodes of realistic sizes are presented.

References:

- [1] Rulin Wang, Yu Zhang, Fuzhen Bi, Thomas Frauenheim, GuanHua Chen and ChiYung Yam, *Nanoscale* 8, 13168 (2016).
- [2] Fuzhen Bi, Stanislav Markov, Rulin Wang, YanHo Kwok, Weijun Zhou, Limin Liu, Xiao Zheng, GuanHua Chen and ChiYung Yam, *J. Phys. Chem. C* 121, 11151 (2017).
- [3] Yu Zhang, LingYi Meng, ChiYung Yam and GuanHua Chen, *J. Phys. Chem. Lett.* 5, 1272 (2014).
- [4] Lingyi Meng, Yu Zhang and ChiYung Yam, *J. Phys. Chem. Lett.* 8, 571 (2017).

二维 IIA/IIB 金属碳化物单层材料电子结构与力学特性

孟令彪

中物院激光聚变研究中心

基于密度泛函理论(DFT)计算与粒子群智(PSO)结构搜索方法,理论设计与预测了 2 维 Mg_2C 与 $\text{Zn}_2\text{C}/\text{Cd}_2\text{C}$ 单层材料稳定结构,计算研究了其电子结构与力学特性。发现 2 维 Mg_2C 单层材料由非常规的 6 配位碳/镁组成,在应力作用下出现金属—零带隙半金属—窄带隙半导体电子结构相变; 2 维 Zn_2C 与 Cd_2C 单层材料具有相似结构,由常规的 4 配位碳组成,呈现较大的纵向褶皱,计算显示体系有非常规的负泊松比,在应力作用带隙可显著变化。独特的电子结构与力学特性使得这些材料有重要的潜在应用。

Electronic structure of cerium based heavy-fermion materials by means of a first-principles many-body approach

Haiyan Lu and Li Huang

Institute of materials, Jiangyou, Sichuan, China

Heavy-fermion materials possess large electronic effective mass due to the scattering by local moments at low temperature and exhibit abundant physical properties because of the c - f hybridization. The complex and subtle interplay between the spin, orbital, and lattice degrees of freedom, as well as the interaction between the strong electronic correlations, large spin-orbit coupling, and intricate crystal-field splitting in these materials, lead to rich quantum phenomena, including heavy-fermion superconductivity, quantum criticality, Kondo effect, and mixed-valence behavior. The archetypical Ce-based heavy-fermion compounds are very sensitive to the change of external environment, such as temperature, pressure, chemical doping, and electromagnetic field, which make them good testing beds for exploring new quantum phenomena and physical mechanisms.

The typical heavy-fermion compounds CeIn_3 , CeB_6 and $\text{Ce}M_2\text{Si}_2$ ($M=\text{Ru, Rh, Pd, Cu, Ag, Au}$) were investigated 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_3 indicates the Ce- $4f$ localized-itinerant crossover with increasing pressure^[1]. The computed electronic structure shows that $4f$ electrons remain incoherent in a broad temperature range of 10 ~ 120 K and $4f$ orbital occupancy, total angular momentum, and total energy exhibit some unusual features near 20 K, suggesting a possible electronic transition^[2]. In addition, the element-dependent electronic structures of heavy-fermion compounds $\text{Ce}M_2\text{Si}_2$ manifest the enhanced localization of Ce- $4f$ upon increasing atomic number. All of these studies enrich the understanding on Ce- $4f$ electronic structure and related physical properties, so as to explore other heavy-fermion systems (such as Sm-, and Yb-based mixed-valence materials) or even the actinide systems (such as the mysterious U-, Pu-, and Am- based strongly correlated materials).

References:

[1] Haiyan Lu and Li Huang, Phys. Rev. B **94**, 075132 (2016).

[2] Haiyan Lu and Li Huang, Phys. Rev. B **95**, 155140 (2017).

高通量材料计算支撑平台 HSWAP 研发进展

肖永浩

中物院计算机应用研究所超算中心

作为“材料基因组计划”的重要一环，高通量材料计算利用超级计算平台，集成高通量材料计算方法 and 系列材料计算软件，可大幅提高新材料筛选效率和设计水平。本文结合高通量材料计算支撑平台 HSWAP 的研发进展，讨论高通量材料计算平台在架构设计、批量关联任务调度、容错/纠错等关键技术及解决方案，最后简要介绍基于 HSWAP 定制的含能材料筛选系统。

Molecular dynamics study of large defects formation induced by displacement cascades in hcp Zirconium

Wei Zhou¹, Jiting Tian¹, Jian Zheng¹, Jianming Xue², Shuming Peng¹

1 Institute of Nuclear Physics and Chemistry, China Academy of Engineering Physics, Mianyang, PR China

2 State Key Laboratory of Nuclear Physics and Technology, School of Physics, Peking University, Beijing, PR China

Large defects are the main factor leading to the degradation of material properties under irradiation environments. Mechanism for the formation of the large defects observable in experiments by displacement cascades in hcp zirconium has been investigated using molecular dynamics simulation. Cascades simulation in the vicinity of the edge dislocation show that a pre-existing edge dislocation can significantly promote the nucleation of the vacancy clusters, and even facilitate the direct formation of an experimental-scale large vacancy loop in only one single displacement cascade. Besides, we perform simulations of cascades overlap in a Zr single crystal at an extremely low temperature. We find that the number of surviving point defects increases and tends to saturate with increasing irradiation dose. Large defects grow gradually and form stable 3D-disordered clusters, which are expected to transform into dislocation loops at a high temperature.

强激光场中的原子分子：基本物理简介以及对数值计算提出的挑战

王旭

中物院研究生院

近年来超强超快激光技术的进展使得强激光场与物质的相互作用成为需要考虑的问题。气态原子分子提供了最简单的研究对象，积累了对这种相互作用过程的理解。我会介绍强激光场与原子分子相互作用相关的基本物理现象和过程，以及这种非微扰性的相互作用对数值计算提出的挑战。最近，强场物理的研究对象开始从气体向固体转变，强场物理与计算材料学可能会有交叉的机会；我会简要介绍一下国际上相关的研究。

钴肟化合物在乙腈-水混合溶剂中催化产氢反应的第一性原理研究

陈金繁

表面物理与化学重点实验室, 江油, 四川

钴肟 (cobaloxime) 配位化合物作为产氢催化剂受到广泛关注, 但其催化反应细节还需进一步研究。本工作中通过第一性原理计算方法 (密度泛函理论和第一性原理分子动力学) 对乙腈-水混合溶剂中的催化产氢过程进行研究, 揭示了溶液中产氢反应的细节和化学基团对催化剂性能的影响, 同时也得出溶剂分子与催化剂的相互作用的信息。我们首先对乙腈-水混合溶剂进行计算模拟, 得到其微观结构的信息。然后, 对几种钴肟化合物 ($\text{Co}(\text{dmgBF}_2)_2$, $\text{Co}(\text{dmgH})_2$, $\text{Co}(\text{dmgH})_2(\text{py})\text{Cl}$) 在乙腈-水溶剂中的产氢过程进行计算模拟, 揭示了产氢体系中质子的输运过程和溶剂分子的作用等。对反应机理的深入认识为设计高效的催化产氢体系提供了有价值的指导。

强关联材料 $\text{La}_2\text{O}_3\text{Fe}_2\text{Se}_2$ 中的电荷与自旋涨落

金光希

中国工程物理研究院，核物理与化学研究所

我们以 DFT+U 方法与 DFT+G 方法研究了强关联材料 $\text{La}_2\text{O}_3\text{Fe}_2\text{Se}_2$ 的电子结构与磁结构。关于此材料的基态磁结构，存在着一些疑问。我们通过 DFT+U 计算，得到的基态磁结构与最近实验所确定的磁结构一致。然而 DFT+U 计算，即使在参数 U 很小的情况下，得到的能隙要远大于实验值 (0.1~0.2 eV)。在此后的 DFT+G 计算中，我们发现该系统电子结构接近于金属绝缘体转变，与实验测量结果相符。根据 DFT+G 计算结果，我们推断此材料的窄能隙性质，与关联作用引起的原子组态涨落密切相关。另一方面，DFT+G 下得到的 Fe 原子磁矩比 DFT+U 下得到的结果要小，这也可以由不同原子组态间的涨落效应予以解释。

References:

- [1] G. Jin, Y. Wang, X. Dai, X. Ren, and L. He, Phys. Rev. B 94, 075150 (2016).

Effect of water in Poly(vinyl formal): Insight from the Molecular Dynamic Simulation

Yin Qiang

Research Center of Laser Fusion, China Academy of Engineering Physics

Polyvinyl formal (PVF, also known as Formvar or Vinylec) is a specialty polymer that possesses a number of desirable properties. Due to its high elongation and ease of fabrication, in particular, the ability to cast it in very thin films, the polyvinyl formal have been used to mechanically support the fuel capsule within the hohlraum in the ignition target which would be planned to produce thermonuclear ignition on the National Ignition Facility (NIF). The positioning of the capsule is critical for a successful experiment on the NIF and the static and dynamic mechanical properties seem to play a crucial role in the positioning of the capsule. In addition, the investigations have been exhibited that polyvinyl formal readily absorbs & desorbs water and high humidity exposure reduces the film strength.

To study the influence of water on the properties of the polyvinyl formal, we performed a series of molecular dynamic simulations to study the water effects on the polyvinyl formal system. We studied the density, fractional free volume, radius of gyration, cohesive energy density, diffusion of water, radial distribution function as a function of content of water. The results show that with addition of water molecular the radius of gyration of the polymer chain decreases whereas the cohesive energy density increases at higher water concentration. These differences resulting from water presence can be attributed to the incorporation of water molecular enhances the intensity of the intermolecular interactions between neighboring macromolecules. The radial distribution function analysis also confirms that the polymer chains form hydrogen bonds with absorbed water molecules, which referred to locate in the vicinity of polar groups on the polymer chains. The simulation results also indicate that the diffusion coefficient of water initially decreased with increasing water concentration but increased beyond a certain value of water concentration. The same change trend also could be found in fractional free volume. These results could be shown that the water molecules appear to be accommodated in the available free volume in the polyvinyl formal matrix at low concentrations, resulting in a decrease in the free volume available to a diffusing penetrant. As the concentration of water is increased, the volumetric swelling of the polymer matrix occurs. All of these results provide molecular insight about molecular structure and physical properties of the polyvinyl formal in different water content.

典型硝基芳香炸药的跨膜运输及其对膜的损伤

周阳

中国工程物理研究院化工材料研究所, 四川绵阳, 621900

以 TNT 为典型代表的硝基芳香炸药能引起中毒性肝病、白内障、高铁血红蛋白症等症状，长期以来被认为对哺乳动物（包括人类）具有细胞毒性。到目前为止，对炸药的跨膜运输的研究几乎没有。因此本文率先采用分子动力学模拟方法研究了 TNT、DNT、MNT 等硝基芳香炸药的跨膜行为及其对膜损伤。结果发现，毒性较强的 TNT，却具有最小的渗透系数；而随着硝基个数的减少，渗透系数在逐渐增加。TNT 在膜中的富集，会导致细胞膜厚度降低；以及富集后 TNT 的跨膜自由能垒急剧降低，这可能是其细胞毒性的重要原因之一。基于此，我们提出了一个 TNT 细胞毒性新机制，即 TNT 在细胞膜中的累积导致细胞膜的损伤机制。这些结果对认识含能材料的细胞毒性具有重要的参考意义。

MOF-5 材料力学与电学性质的第一原理计算

王晓媛

中物院总体所

利用基于密度泛函理论的第一原理计算的方法研究了典型金属有机框架材料—MOF-5 的力学、电学性质及其机电耦合特性。通过对 MOF-5 材料施加不同类型的外部载荷，获得了 MOF-5 的弹性常数、杨氏模量等基本力学参数。另外，利用能带结构分析等研究了 MOF-5 的本征电学特性，发现 MOF-5 的禁带带宽为 3.49 eV，属于宽禁带半导体。对 MOF-5 电学性质的机电耦合特性研究发现，外界应变会显著降低 MOF-5 的禁带带宽，提高其导电性。通过进一步分析其电子态密度、共价键键长等的变化，发现外界应变会引起 MOF-5 有机配体中共价键强度的降低，继而导致材料禁带带宽的减小。研究从理论上定量揭示了外部应变对 MOF-5 电学性质的影响，为基于 MOF-5 的气氛传感器优化设计和性能评估等提供了重要的理论基础。

Phase stability of UT_2Al_{20} (T=Mo,Nb,Ti,Zr) and electronic structure

Xin Wang, Pengchuang Liu, Yajiang Xian, Pengcheng Zhang

Institute of Materials, China Academy of Engineering Physics, China

In this talk, the phase stability of UT_2Al_{20} (T=Mo,Nb,Ti,Zr) was explored using cluster formula in combination with first-principles calculations. Cluster formula analysis uncovered that the compound was composed of two principal clusters, i.e. $[T-Al_{12}]$ and $[U-Al_{16}]$. The electronic interactions between U, T and Al atoms in this compound were discussed using elastic property, Bader charges and energy-resolved local bonding analysis, as well as the electronic interactions between T and Al atoms in $[T-Al_{12}]$ cluster and between U and Al atoms in $[U-Al_{16}]$ cluster. It revealed that UT_2Al_{20} satisfied the mechanical stability criterion for cubic system, and exhibited near ionic bonding character with weak bonding directionality. The calculations within both standard DFT and HSE frameworks demonstrated that U and Al atoms acted as an electron donor while T atoms acted as electron acceptor. The intrinsic stability of UT_2Al_{20} mainly stemmed from the bonding states of T-Al bonds and Al-Al bonds in $[T-Al_{12}]$ cluster. These calculations provide a further insight on the $CeCr_2Al_{20}$ -type ternary compounds.

References:

- [1] Peng-Chuang Liu, Ya-Jiang Xian, XinWang*, Yu-Ting Zhang, Peng-Cheng Zhang. J.Nucl. Mater., 493 (2017) 147-153











