基于原子择优占位的高熵合金（高熵材料）四大效应的定量化计算和图像化表征

系列方法线上&线下实战研修班通知

Series of Practical Training Seminars for

Quantitative calculation and graphical characterization of four Core effects of high entropy alloy (high entropy materials) based on atomic site preference

(General Flyer)

时间 Date：（按需开展线上/线下教学,早学早用，人数不限少）

春季班：3 月 27-30 日；寒假班 1 月 8-14 日

初夏班：5 月 7-10 日;暑期班：7 月 16-21 日;秋季班：11 月 1-4 日;）

(一次注册，长期线上保驾护航，直至论文发表),

方式 Way：线上线下同步讲课，云计算展播、训练和 QQ 远程协助相结合(Combination of online course,cloud computing demonstration, training and remote personal assistance)

主办：福州大学多尺度材料设计与应用实验室 http://mcmf.fzu.edu.cn

承办：福州博德新材料科技有限公司 www.bode-tech.cn

协办：北京并行科技有限公司 (助您分分钟驶入计算快车道，24 小时在线贴身保驾护航，点击试用）

Host: Multi-scale Computational Material Facility, School of Materials, Fuzhou University

Co-organized: Fuzhou Bode Advanced Material Co., Ltd. **Beijing Parallel Technology Co., Ltd.**

注册费：寒假班，暑假班 3000 元/人 (含 500 元机时费，如学员负责自己的超算资源，则注册费 2500 元)。

Registration fee: 600$ for DEVELOPED country register (save 100$ if using own supercomputer resource)

春季班；初夏班;秋季班;2500 元/人）(含 500 元机时费，如学员负责自己的超算资源，则注册费 2000 元)。

高熵合金（高熵材料）计算模拟专题培训咨询 QQ 群: 183881047

吴波教授：QQ:654489521@qq.com,电话：13023819517 首席教学和科研负责人

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1.达成目标

基于晶体结构模型构筑合金热力学模型，结合相平衡和第一性原理计算，完成各种结构的高熵合金（高熵材料）（单相为主）四大效应的定量化和图像化表征。

计算零基础学员，完成一个自己选定的高熵合金（高熵材料）体系，对其结构和性质进行全流程定量化和图像化表达，包含自主建模、热力学数据库构建、占位分数计算、基于占位分数的原子分布模型构建、短程有序或局域有序化团簇，点阵常数、晶格畸变驱动力及畸变率，弹性各向异性力学性质、韧脆性、间隙原子扩散、初步了解高熵合金（高熵材料）的催化特性建模和计算分析之定量化和图像化表达。没出论文初稿，不准走人（包教包会，长期在线辅导,疫情平稳后，欢迎到福州江景 SOHO 现场作文，或吴波教授受邀到贵单位走访辅导）

1. Achieve your goals

Based on crystal structure model,building alloy thermodynamics, by combing computational thermodynamics and first-principles calculations, the four core effects of high entropy alloys with various structures (single phase) were quantitatively and graphically characterized.

Students practice a self-selected high entropy alloy, achieve independent modeling, thermodynamic database construction, site occupying fractions calculation, atomic distribution model construction based on site occupying

fractions, short range ordering(SRO) or local ordering, diverse mechanical property calculation, interstitial atom diffusion, and preliminary understanding of catalytic characteristic modeling and calculation analysis of high entropy alloy. (Online consult and help are available till well grasping)

预报名表接收邮箱： info@bode-tech.cn, fzu_mcmf1@sina.com, wubo@fzu.edu.cn
Register Form please Email to info@bode-tech.cn, fzu_mcmf1@sina.com, and wubo@fzu.edu.cn

授课咨询 Consult for teaching course：吴波 教授(Prof. Wu）13023819517(微信）wubo@fzu.edu.cn
会务助理 Consult for training service：吴睿 先生 13691685245（微信）
课堂入口信息：开课前发送内部授课资料和腾讯会议登录信息到报名邮箱
Classroom entrance information: The teaching materials and Tencent conference login information will be emailed to the registration mailbox before the class starts

备注：原则上应自备 VASP\PHONOPY\热力学软件版权或申请试用版，或以适当方式合作
Remarks: In principle, you should bring your own VASP\ PHONOPY\ thermodynamic software copyright or apply for a trial version，or cooperation properly

2.需求分析

高熵合金（高熵材料）是一种划时代的材料设计理念，不少材料具有一种或多种潜在的优异性能，由此也启发人们提出了**各种各样高熵材料新概念，频频艳羡于《Nature》 &《Science》，此乃高熵合金幸事和盛世**。与此同时，高熵合金（高熵材料）存在很多争议，甚至连高熵合金这个名字都被不少有识之士避而不谈。广为人知的高熵合金（高熵材料）的四大效应（热力学上的高熵效应，动力学上的迟滞扩散效应，结构上的晶格畸变效应，性能上的鸡尾酒效应），也不时受到质疑，因为随便一种效应，都很容易被人举出反例而显得尴尬，说明高熵合金（高熵材料）的合金化理论研究（结构与性能的关系）还很不充分。另一方面，合金成分组合海量，如何钓到大鱼，烧钱式广泛撒网并不可取，也不可能。与其临渊羡鱼，不如退而结网，把基础方法搞通再出海。基于材料基因工程理念，运用高通量实验，尤其是借助高通量计算，积累海量数据后辅助以机器学习的 AI 材料设计是必由之路。

考虑到组成高熵合金（高熵材料）的原子种类众多，各种组成原子结构和性质各异，FCC，BCC 和 HCP 也呈现出迥异的晶体结构，因此，原子在亚晶格和整体晶格上必然存在择优占位行为（占位有序化行为，site preference），而**基于传统的随机固溶体模型方法的 SQS 及 CPA-EMTO 似乎不能描述真实合金体系的结构特性，既抹杀了组成原子种类差异，也抹杀了合金相结构差异，并且还忽略了热处理温度的影响，用 S=Rln(n) 描述构型熵，这只代表了实际并不存在的那种最理想的原子排布模式。**因此，将复杂的高熵合金（高熵材料）简单化描述，感觉不一定站得住脚。高熵合金（高熵材料）研究开发已发展到新阶段，有必要也有可能进行理性化描述。

基于以上理性思考和实践，吴波等人经过多年前期探索，创新性地建立了一系列定量化和图像化描述高熵合金（高熵材料）的四大效应的理性方法，系列方法论学术论文和专利发表后，引起同行较大关注，收到不少热情鼓励和诚恳建议，也收到不少的学习咨询，期望提供学习和计算模拟实战机会。新冠疫情复杂多变期间，高熵材料发展不停步，学术论文仍一日见刊 10 篇以上，不乏 N&S 大刊。研究者对该领域的新方法和新想法必须密切跟进，才能有高质量的科研成果。因此，本系列培训应需而为，以期为同行提供一些理性思路和新方法。

2. Requirements analysis

High entropy alloy is an epoch-making alloy design concept. Many alloys may have one or more potential excellent properties, which also inspires people to put forward various new concepts of high entropy materials. **High impact papers are emerging every day, even highlighted in 《Nature》 and 《Science》, thus it is a Booming Times of HEAs**. However, there are many controversies about high entropy alloy, and even the name of high entropy alloy has been avoided by many people of insight. The four well-known effects of high entropy alloy (high entropy effect in thermodynamics, sluggish diffusion effect in kinetics, sever lattice distortion effect in structure and cocktail

effect in performance), It is also questioned from time to time, because any kind of effect is easy to be cited as a counterexample, which shows that the alloying theory research (the relationship between structure and properties) of high entropy alloys is still insufficient. On the other hand, there are a large number of alloy compositions, so it is neither advisable nor possible to catch big fish and burn money to cast a net widely. It is wisdom to find a reasonable reliable and general simulation approach at first. Artificial Intelligent Materials Design (AI-MD) is the future way based on the concept of material genetic engineering, by employing high-throughput experiments, especially high-throughput calculations, assisting machine learning after accumulating massive data.

Considering that there are many kinds of atoms that make up high entropy alloys, different kinds of constituent atoms have different structures and properties, FCC, BCC and HCP also show different crystal structures, Therefore, atoms must have preferred site preference on sublattice and global lattice. However, **SQS and CPA-EMTO based on the traditional random solid solution model method can't describe the structural characteristics of real alloy system. They not only ignore the differences of composition atoms, but also ignore the differences of alloy phase structure, and even ignore the effect of heat treatment temperature on the site preference, thus S=Rln (n) is used to describe the configuration entropy, which only represents the most ideal atomic arrangement mode that does not exist in practice.** Therefore, it may not be tenable to simplify the description of complex high entropy alloys. The research and development of high entropy alloys has developed to a new stage, so it is necessary and possible to describe them rationally.

Based on the above rational thinking and practice, Prof. Dr. Wu Bo and others colleagues put forward a series of methods to describe the four effects of high entropy alloy quantitatively and graphically after many years of early exploration. After the publication of a series of methodological academic papers and patents, they attracted great attention from peers and received many peer comments and consultations, expecting to provide sharing and teaching opportunities. There are still 10 complex and high-entropy academic papers in COVID-19 pandemic every day, including published in **《Nature》** and **《Science》**. Thus, new methods and ideas in this field must be closely followed up in order to have high-quality scientific research results. Therefore, this series of training should be needed to provide some new ideas and methods for peers.

3.课程之学术思想及讲授提纲（讲课和上机实践安排表细化后公布）

- 高熵合金（高熵材料）理论研究进展述评　高熵合金（高熵材料）计算模拟方法述评
- **第一性原理计算方法快速入门　计算热力学与相平衡快速入门**
- 高熵合金（高熵材料）有序化结构建模，高熵合金（高熵材料）合金热力学描述
- 端基热力学数据库构筑，相比例、相成分、占位分数计算
- 基于占位分数的原子分布模型搭建
- 平衡态下局域有序结构定量化和图像化表征
- 晶格畸变驱动力及晶格畸变率定量化和图像化表征
- 高熵合金（高熵材料）电子结构分析
- 高熵合金（高熵材料）**基态**及**高温力学性能**预测
- 间隙原子扩散能垒波、扩散常数、扩散系数计算
- 高熵合金（高熵材料）表面能，表面吸附
- 高熵合金（高熵材料）催化建模、计算与分析初步

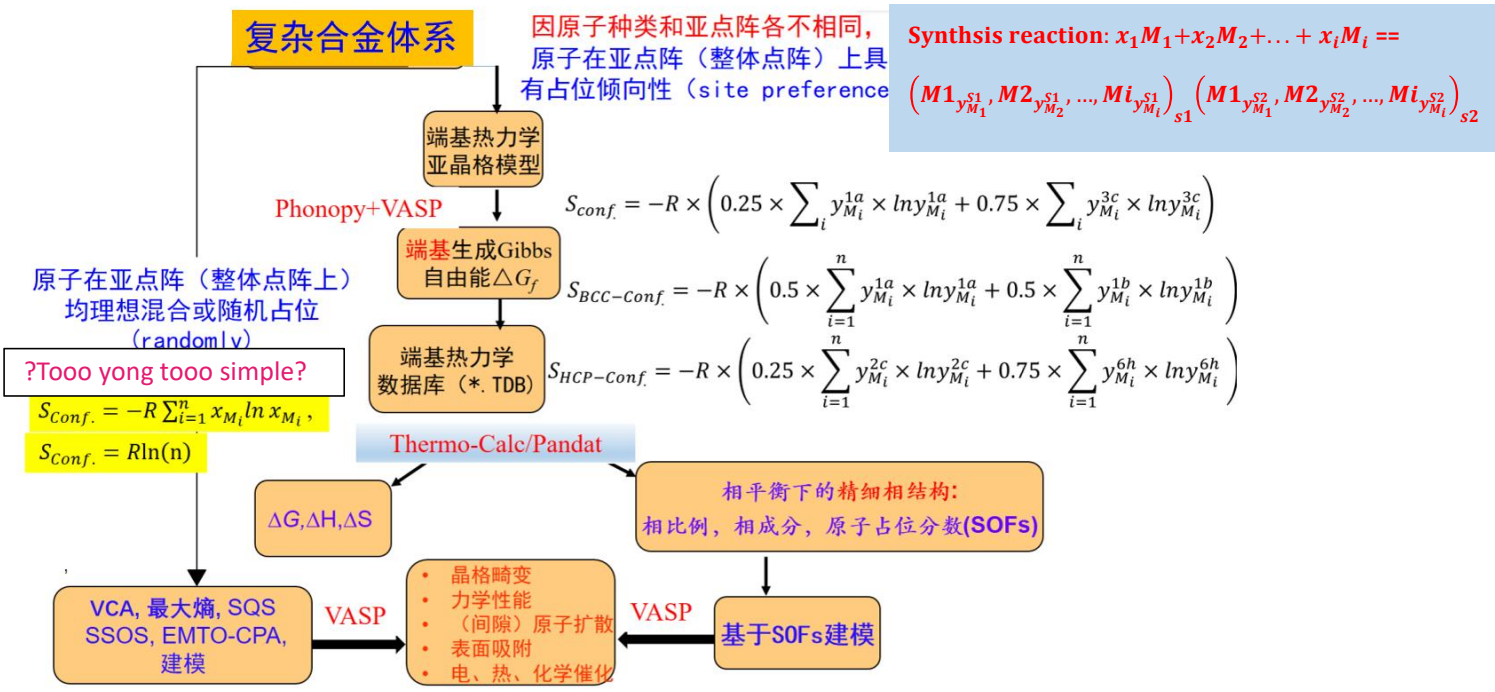

Fig. 3-1. Academic innovative and research flow chart of complex alloy phase with site occupying fractions.

3. Schedule of course teaching, modeling and computer calculation

(1) Review on the theoretical research progress of high entropy alloys

(2) A quick start to First-principles computing methods

(3) A Quick start to computational thermodynamics and phase equilibrium

(4) Description of calculation and simulation methods for high entropy alloys

(5) Ordered structure modeling of high entropy alloys （high entropy materials）

(6) Thermodynamic description of high entropy alloy（high entropy materials）

(7) Construction of end-based thermodynamic database of high entropy alloys （high entropy materials）

(8) Calculation of phase proportion, phase composition and occupying fraction

(9) Establishment of atomic distribution model based on occupying fraction

(10) Quantification and image characterization of Local ordered structures in equilibrium state

(11) Electronic structure analysis of high entropy alloy（high entropy materials）

(12) Prediction of mechanical properties of high entropy alloys（high entropy materials）

(13) Calculation of diffusion energy barrier wave, diffusion constant and diffusion coefficient of interstitial atoms

(14) Surface energy, surface adsorption of high entropy alloy（high entropy materials）

(15) Preliminary modeling, calculation and analysis of high entropy alloy catalysis

4. 高熵合金（高熵材料）计算培训报名登记表 Register form

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（酌情填写有关信息）

姓名 Name	
单位 affiliation	
学员类别 Academic degree level （本科生、硕士生、博士生、教师）+（在读生导师姓名）	
性别 (Sex)	
Email address	
联系电话	
联系 QQ	
微信号	
有无 VASP 经验 experience of VASP	
有无热力学软件经验 experience of comput. thermodynamics	
拟解决的主要问题 main puzzle	
发票类型（会议费，培训费，计算服务费，加工费，测试费等）（提供单位名称和统一社会代码识别号）	
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地址：福州高新区福州国家留学人员创业园 公司网址：www.bode-tech.cn

Paypal account : lmhuadr@gmail.com

附：其他参考资料

5.学术积累

（1）科研项目

Proj.1. 高熵合金形成的热力学原理和成分设计新方法探索 （国自然面上项目）

Proj.2. 金属间化合物中合金元素的占位有序化行为研究 （国自然面上项目）

Proj.3. 高铁、高铝低成本高熵合金的热力学、成分和性能优化设计研究 （教育部博导基金）

Proj.4. 耐蚀、高弹、磁性高熵合金的设计、制备与性能研究 （省自然面上项目）

Proj.6. FCC 高熵合金设计新原理和新方法研究 （省人才项目）

Proj.7. 含 Fe、Co、Ni 五组元 FCC 结构高熵磁性合金成分数据库的设计研究及制备

Proj.8. 耐腐和高弹性的多主元高熵合金设计方法和数据库研究

（2）专利 Patents

[1] ZL2021100207115 基于原子占位有序化行为的高熵合金构型熵的计算方法，发明专利，免答辩授权

[2] ZL2020112307425 基于原子占位有序化行为的高熵合金晶格畸变量计算方法，发明专利，免答辩授权

[3] ZL2021100169842 一种间隙原子在高熵合金中的扩散行为的计算方法，发明专利，小修后已授权

[4] 2020112947690 基于原子在亚晶格占位行为的高熵合金力学性能计算方法，实质审查生效

[5] 2022111038083 一种基于 Python 的原子配位数自动化批量计算统计方法，实质审查生效

[1] ZL2021100207115, Calculation method of configuration entropy of high entropy alloy based on atomic occupation ordering behavior, Granted invention patent

[2] ZL2020112307425, Calculation method of lattice distortion of high entropy alloy based on atomic occupation ordering behavior, Granted invention patent

[3] ZL2021100169842, A method for calculating the diffusion behavior of interstitial atoms in high entropy alloys, Granted invention patent

[4] 2020112947690, Calculation method of the mechanical properties of high entropy alloy based on the occupation behavior of atoms in sublattice, substantive examination takes effect, 1st-turn defence response

[5] 2022111038083, An automatic batch calculation statistical method of atomic coordination number based on Python, substantive examination takes effect

（3）论文 Academic papers

[1] Bo Wu* , Yan Zhao* , Hamid Ali, Rong Chen et al. , **A reasonable approach to describe the atom distributions and configurational entropy in high entropy alloys based on site preference**, *Intermetallics* 144 (2022) ,May, 107489. https://doi.org/10.1016/j.intermet.2022.107489（The Most Downloaded Articles in 《Intermetallics》 in the last 90 days (May--September,2022)

【论文中文解读：
https://mp.weixin.qq.com/s?__biz=MzIzMTUzMDk4Mw==&mid=2247484134&idx=1&sn=b0136482fab4a2bd71b0766243aafcba&chksm=e8a38a6edfd40378ac65c2e43ab3da29e11747444d2d5867124c6c9220dc135c058a416fbd9e&cur_album_id=2697658112350339074&scene=189#wechat_redirect】

[2] Rong Chen, Hamid Ali, Bo Wu* , Yan Zhao, et al., **A general approach to simulate the atom distribution, lattice distortion, and mechanical properties of multi-principal alloys based on site preference: using FCC_CoNiV and CoCrNi to demonstrate and compare,** *Journal of Alloys and Compounds,* 2023, 935(1):168016, https://doi.org/10.1016/j.jallcom.2022.168016.

【论文中文解读：https://mp.weixin.qq.com/s/vttSf75_UF0eTnTZlMUFxg 】

[3] H. Ali, R. Chen, B. Wu*, T. Xie, L. Weng, J. Wen, Q. Yao, L. Su, Y. Zhao, P. Zhao, B. Sa, Y. Liu, C. Wang, H. Su, A. Hayat, **The site preference and doping effect on mechanical properties of Ni_3Al based γ′ phase in superalloys by combing first-principles calculations and thermodynamic model,** *Arabian Journal of Chemistry*. 15(11) (2022) 104278, https://doi.org/10.1016/j.arabjc.2022.104278

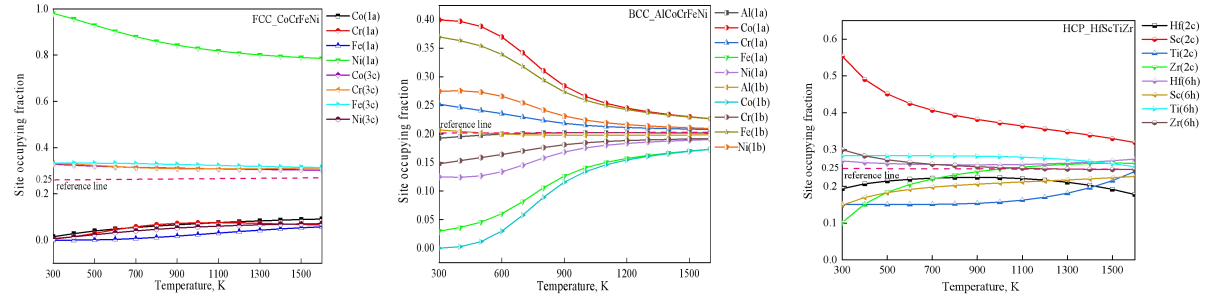
[4] H. Ali, R. Chen, H. Chen, Y. Zhao, P. Zhao, S. Yang, B. Wu*, J. Wen, C. Zhang, L. Weng, T. Xie, Q. Cai, L. Zhang, Z. He, Q. Yao, H. Zhang, B. Sa, C. Wen, C. Wang, **The Ordering Behavior of Co_3Al-based γ′ Phase with $L1_2$ Structure Predicted by the Thermodynamic Model with Support of First-principles Calculations**, *Materials Today Communications*. 33 (2022) 104447, https://doi.org/10.1016/j.mtcomm.2022.104447

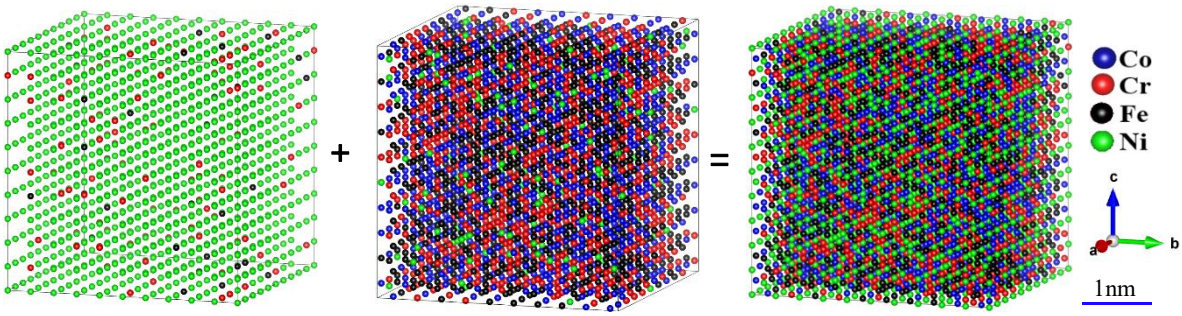
[5] Bo Wu* , Zheyu Xie, Jinchang Huang, Jinwei Lin, Yixu Yang, Linqiao Jiang, Jianglin Huang, Guoxin Ye, Chunfeng Zhao, Shangjin Yang, Baisheng Sa, **Microstructures and thermodynamic properties of high-entropy alloys CoCrCuFeNi**, *Intermetallics* 93 (2018) 40–46. , https://doi.org/10.1016/j.intermet.2017.10.018

[6] 谢哲宇，吴 波* ，黄锦长，杨义许，李皎亮，**多主元高熵合金 MoNbTaVW 中合金元素的占位行为**，中国科技论文在线精品论文（博士点基金博导类结题指定在线发表论文）

[7] Zhang C, Lin M, Wu B et al. **Explore the Possibility of Forming fcc High Entropy Alloys in Equal-Atomic Systems CoFeMnNiM and CoFeMnNiSmM**. *Journal of Shanghai Jiaotong University (Science)*, 2011, 16(2):173-179.

6.图文案例





1a sublattice in 10×10×10 supercell　　3c sublattice in 10×10×10 supercell　　10×10×10 supercell of FCC structure

$(Co_{0.0705}Cr_{0.0750}Fe_{0.0229}Ni_{0.8316})_{1a}$ + $(Co_{0.3098}Cr_{0.3083}Fe_{0.3257}Ni_{0.0562})_{3c}$ = $(Co_{0.0705}Cr_{0.0750}Fe_{0.0229}Ni_{0.8316})_{1a}$ $(Co_{0.3098}Cr_{0.3083}Fe_{0.3257}Ni_{0.0562})_{3c}$

$Co_{71}Cr_{75}Fe_{23}Ni_{831}$ + $Co_{929}Cr_{925}Fe_{977}Ni_{169}$ = $Co_{1000}Cr_{1000}Fe_{1000}Ni_{1000}$

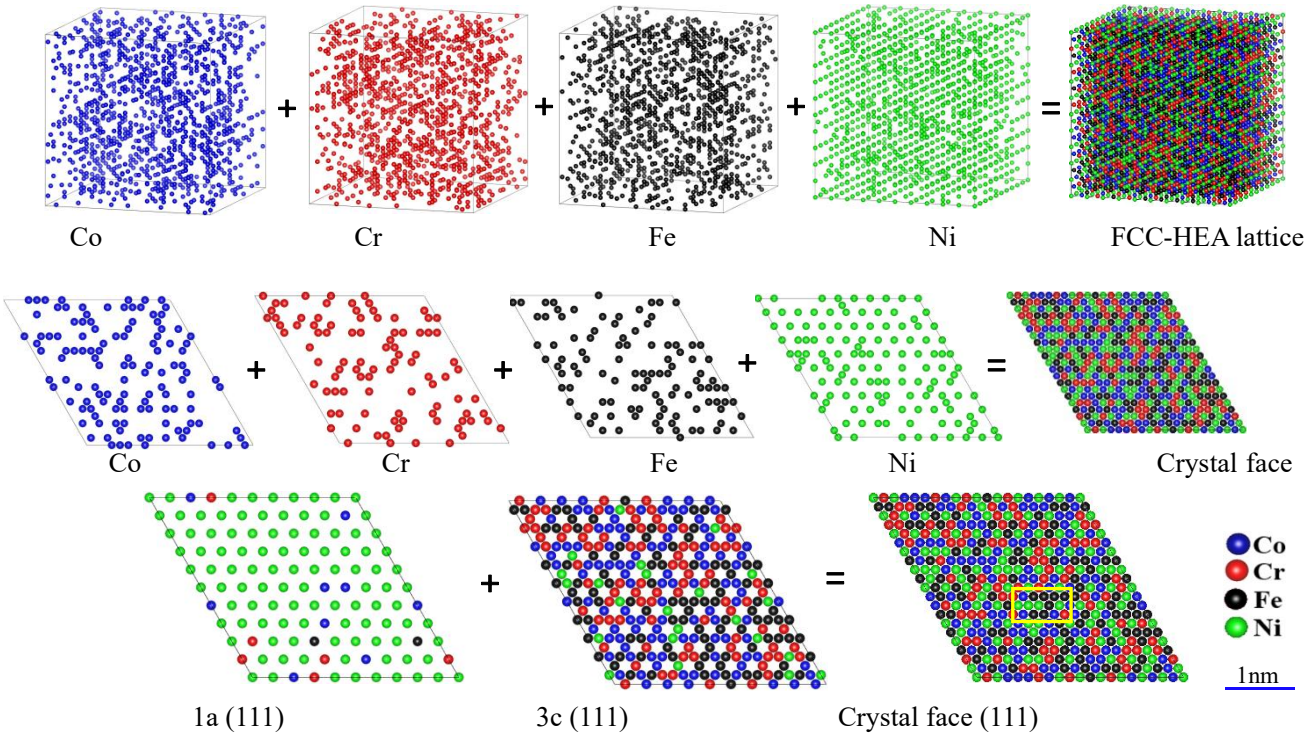


Fig. Visualization of atomic distribution with the real relative size on the sublattice 1a and 3c, as well as on the full FCC lattice for FCC_CoCrFeNi HEA subjected to heat treatment to equilibrium at 973K

The site preference of atoms is considerably strong. For the CoCrFeNi high entropy alloy with FCC phase structure, Ni strongly favors 1a sublattice, and the Co, Cr, and Fe prefer to 3c sublattice when the phase reaches its equilibrium at 973K. The local ordered cluster is identified directly.

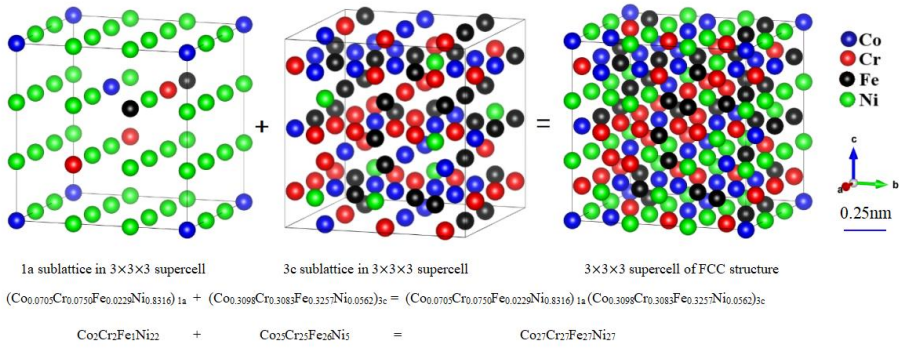
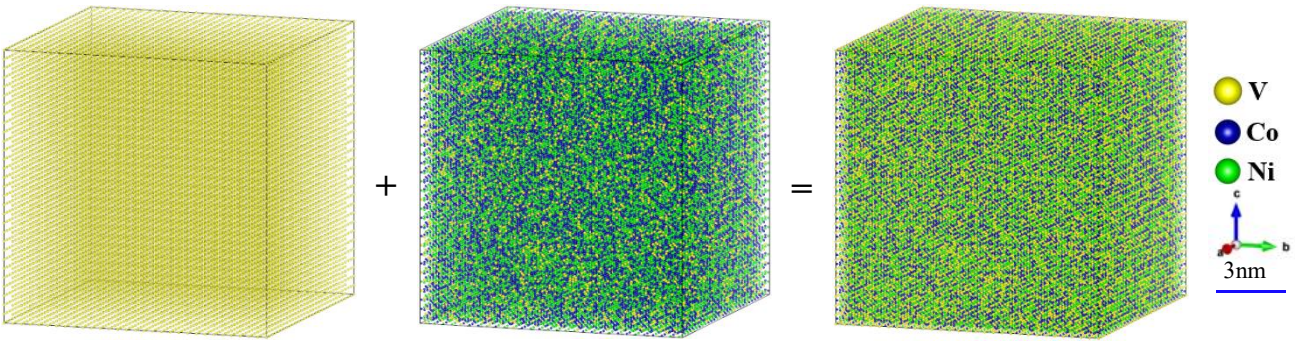


Fig. 7 Construction of a 3×3×3 FCC supercell for FCC_CoCrFeNi HEA with sublattice nested at 973K

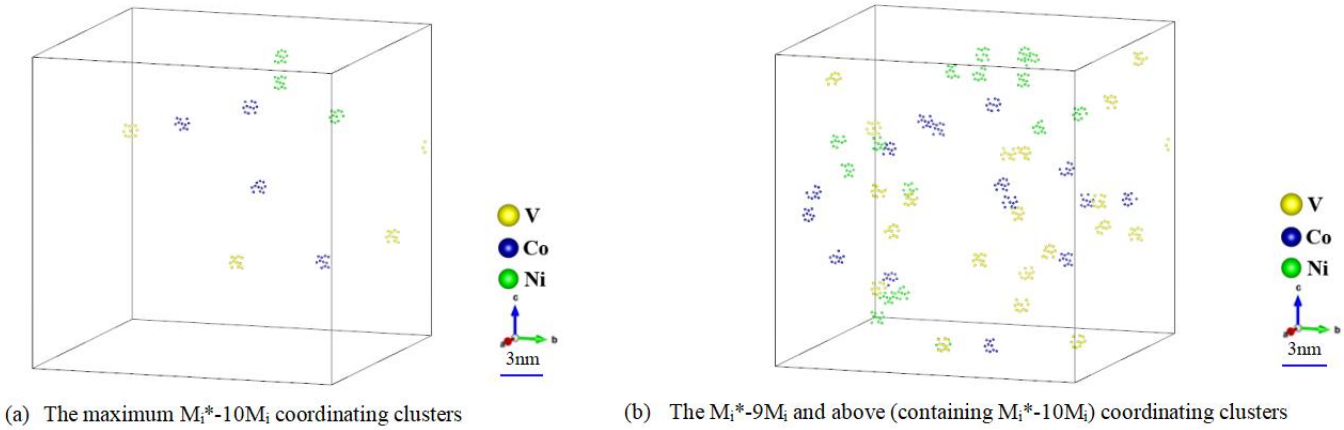


1a sublattice in 30×30×30 supercel 3c sublattice in 30×30×30 supercell 30×30×30 supercell of FCC structure

$(V_{1.0000})_{1a}+(Co_{0.4445}Ni_{0.4444}V_{0.1111})_{3c}= (V_{1.0000})_{1a}(Co_{0.4445}Ni_{0.4444}V_{0.1111})_{3c}$

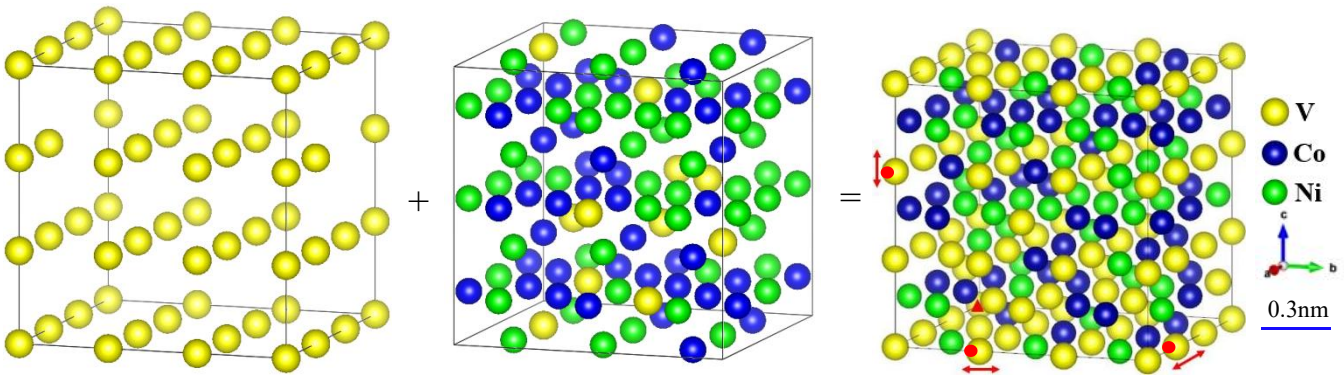
V_{27000} + $Co_{36000}Ni_{36000}V_{9000}$ = $Co_{36000}Ni_{36000}V_{36000}$

(c) Construction of a 30×30×30 FCC supercell based on the prototype of $L1_2$_$AuCu_3$ for FCC_CoNiV MEA at all temperature



(a) The maximum M_i*-10M_i coordinating clusters (b) The M_i*-9M_i and above (containing M_i*-10M_i) coordinating clusters

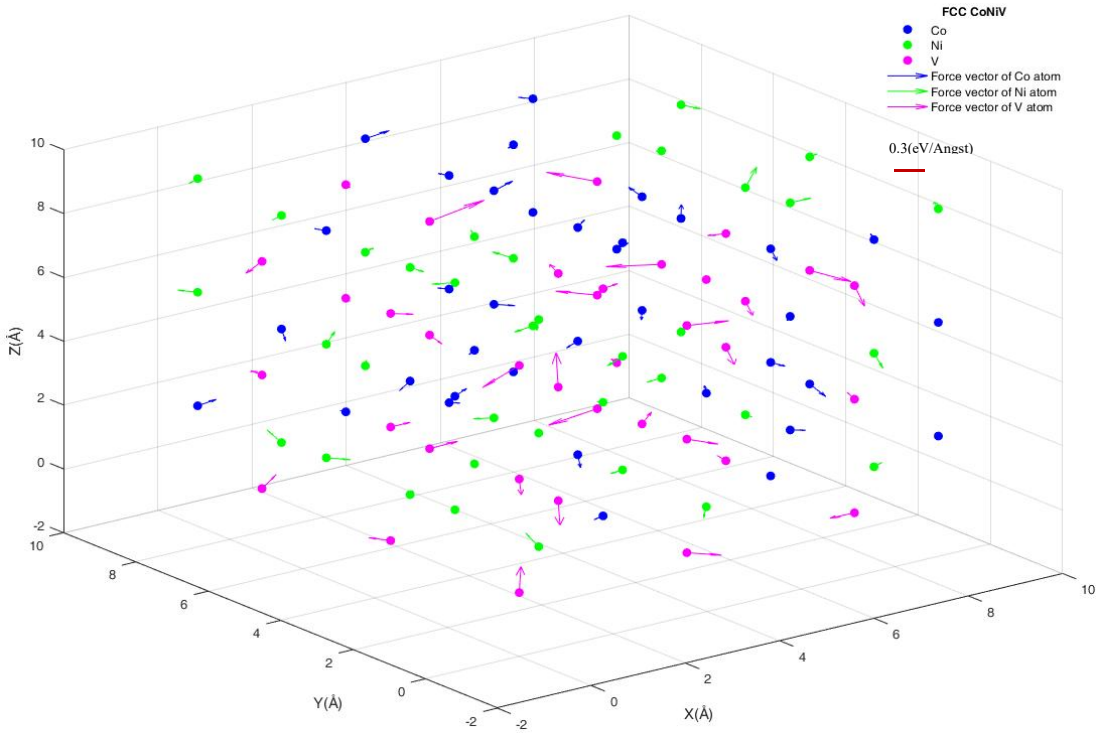
Fig. 11. The maximum M_i*-10M_i coordinating clusters in a hypothesized randomly mixing configuration of FCC_CoNiV MPA with a 30×30×30 FCC supercell based on the prototype of $L1_2$_$AuCu_3$ containing 108,000 atoms



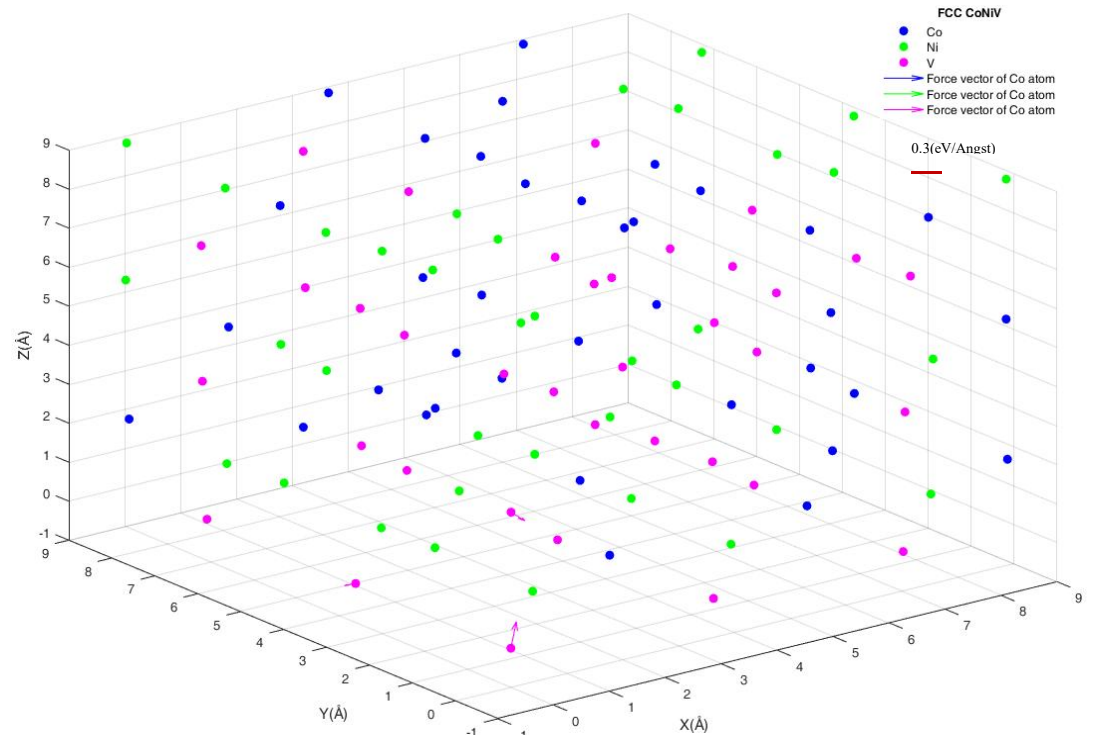
$(V_{1.0000})_{1a}+(Co_{0.4445}Ni_{0.4444}V_{0.1111})_{3c}=(V_{1.0000})_{1a}(Co_{0.4445}Ni_{0.4444}V_{0.1111})_{3c}$

$(V_{27})_{1a}$ + $(Co_{36}Ni_{36}V_9)_{3c}$ = $(V_{27})_{1a}$ $(Co_{36}Ni_{36}V_9)_{3c}$

Fig. 12 A3×3×3 FCC supercell based on the prototype of $L1_2$_$AuCu_3$ containing 108 atoms for FCC_CoNiV MPEA used to fulfill first-principles calculation based on the available computer power.



(a) Driven force of lattice distortion analyzed from the resultant force acting on each atom of the FCC_CoNiV MPEA without lattice distorting after volume relaxing only (R7)



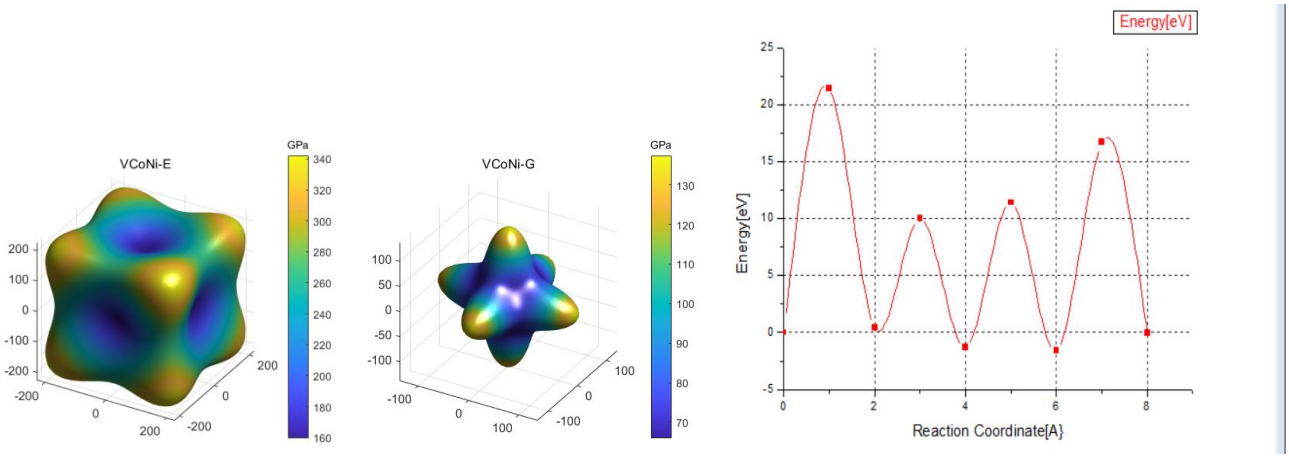
(b) Driven force of lattice distortion analyzed from the resultant force acting on each atom of the FCC_CoNiV MPEA with lattice distorting by full relaxing (R3, volume, shape and atom positions were allowed to relax)

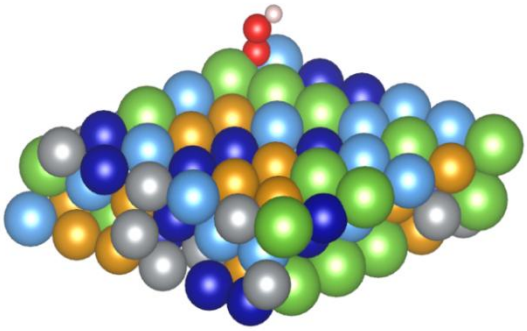
Fig. 16. Driven force of lattice distortion analyzed from the resultant force acting on each atom of the FCC_CoNiV MPEA with and without lattice distortion based on the SOFs at 973 K

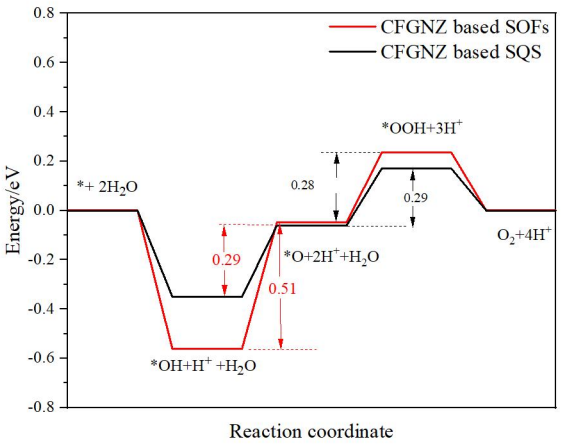
Other advanced calculation and characterization such as

- Electronic Structure with DOS, pDOS,Chemical bond, Electronic local function (ELF), charge map,
- Anisotropy mechanical properties characterized quantitatively and intuitively,
- Check and verify the exact cocktail effect,
- Barrier wave and coefficients of interstitial atom diffuse,
- Surface properties
- Absorption of some definite surface
- Catalytic properties
- Miscellaneous ...

+specially welcome the Puzzles to explore from students in due course.







+Many interesting results to share!

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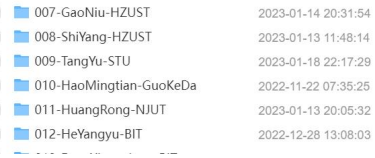
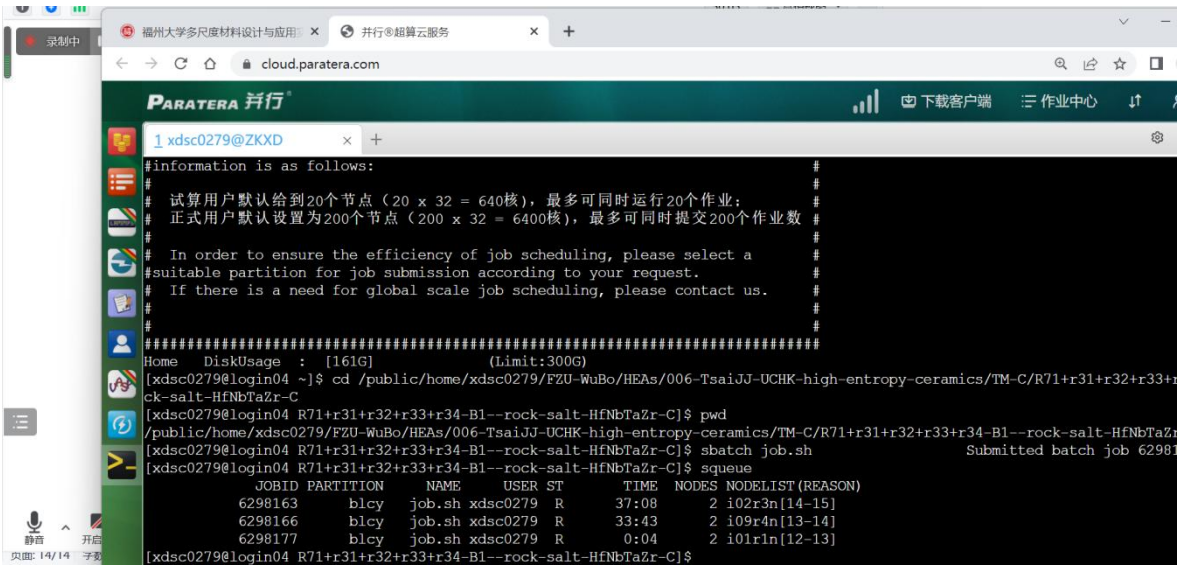
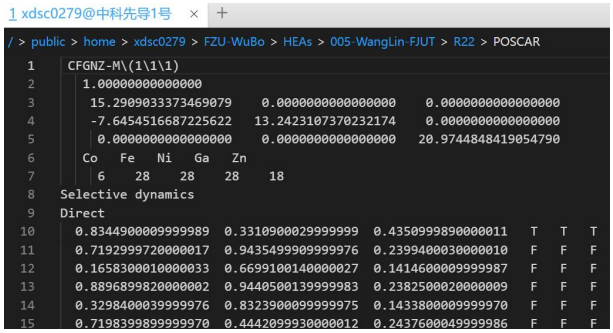
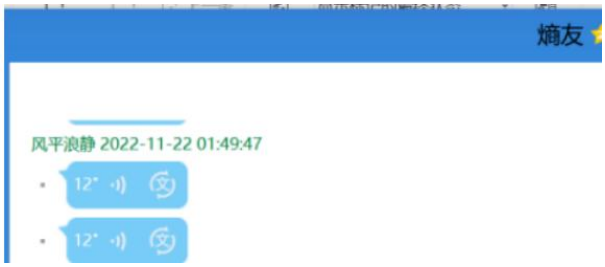
Glace the solution of the scheduled Online training in this special occasion 已授课展示

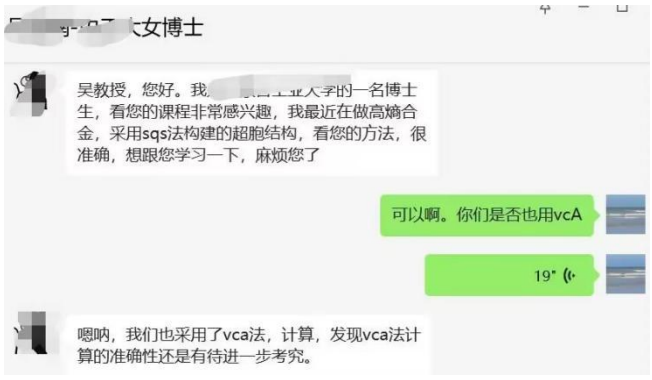






知音可贵！一对一辅导与交流，热爱学习的都是大有希望的好学生。





风平浪静(654489521) 13:24:55
部分同学进展和理解掌握很不错，说明本身不难，大家相互学习，
风平浪静(654489521) 13:26:17
其中，福建师大吕明月 0 基础起步，跑得比我快，可以交个学友
风平浪静(654489521) 13:26:23
吕明月-福师大(1610034962) 13:31:37
主要是老师讲的好，视频录的很清晰，可以反复学习，我才看了一点点，
还有好多好多都还没学，以后还要多多学习，谢谢老师

上善若水 三金男-上海大学 2022-12-25 21:29:39
我向导师汇报了试听您几次的授课情况，导师非常鼓励我向您学习，我已经报名参加了咱们的培训课程，希望掌握高熵合金前沿计算模拟方法，多出好成果。很期待，老师辛苦啦！

风平浪静 2022-12-25 21:40:03
欢迎

学员任务进程表（阶段性自我对照表）汇报日期 2023-01-28												
学习内容	1.引言：计算模拟背景理解	2.第一性原理全流程-r31-r3f-dos-band-optics-E-V	3.端基声子热力学计算	4.端基声子热力学G(T)多项式拟合	5.数据库构建（至少会在模板上替换一个端基）	6.占位分数SOFs计算，构型熵定量化计算	7.基于占位分数SOFs高熵合金POSCAR结构模型，统计团簇，短程序	8.高熵合金POSCAR-r7-r7+r3晶体结构优化计算及晶格畸变分析	9.对于平衡体积左右偏离，不同体积下总能计算，拟合状态方法获得体积弹性模量B	10.Cij（弹性系数矩阵计算-参考2009吴松文档）	11.基于块体POSCAR，用VESTA转换出*.cif,用Materiasl Studio切出表面，吸附，催化初探	12.学术论文构思和撰写（题目，框架，前言选题，素材积累，句段积累及成文情况）
吕明月-福师大	√	√	√	√	√	√	√	√	√	√	doing	doing
高妞-华中科大	√	√	√	√	√	√	√	√	√	to do	doing	doing

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