

## **2019 机器学习-计算化学 Workshop**

固体表面物理化学国家重点实验室

**主办单位:** 福建省理论与计算化学重点实验室

厦门大学化学化工学院

**组委会委员:** 程俊 吴玮 吕鑫 赵仪  
曹泽星 梁万珍 王斌举 苏培峰



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## 2019 机器学习-计算化学 Workshop 日程表

地点：化学报告厅/同安二 106

Date	Morning (化学报告厅)			Afternoon (同安二 106)	
3 <sup>rd</sup> Sept.				14:00-20:00	Registration at Lujiaxi Building (卢嘉锡楼大厅)
4 <sup>th</sup> Sept.	08:15-08:30 Opening <b>Section 1</b> Chair: Jun Cheng (程俊)			14:00-15:50	<b>Tutorial: SOAP/GAP</b> Tutors: Gábor Csányi, Jianxing Huang (黄剑兴), Feng Wang (王锋)
	08:30-09:30 Advances in interatomic potentials for materials Gábor Csányi, University of Cambridge				
	09:30-10:30 Global Neural Network Potential from Construction to Simulation Zhipan Liu (刘智攀), Fudan University				
	10:30-10:50 Photo/Break			15:50-16:10 Break	
	<b>Section 2</b> Chair: Binju Wang (王斌举)			16:10-18:00	<b>Tutorial: LASP</b> Tutors: Zhipan Liu (刘智攀), Cheng Shang (商城), Yunpei Liu (刘云霈)
	10:50-11:50 Ab initio thermodynamics with the help of machine learning Bingqing Cheng (程冰清), University of Cambridge				
	11:50-12:20 Integrating Machine Learning and Molecular Modelling for Drug Design Jianing Lu (卢佳宁), New York University				

5 <sup>th</sup> Sept.	<b>Section 3</b> Chair: Yi Zhao (赵仪)	08:30- 09:30	<b>Deep Learning for Multi-Scale Molecular Modeling</b> Linfeng Zhang (张林峰), Princeton University	14:00- 15:50	<b>Tutorial: DPMD</b> Tutors: Linfeng Zhang (张林峰), Yuzhi Zhang (张与之), Jianxing Huang (黄剑兴), Yongbin Zhuang (庄永斌), Feng Wang (王 锋)
		09:30- 10:30	<b>Data-Driven Materials Discovery with the Method SISSO</b> Runhai Ouyang (欧阳润海), Shanghai University		
	10:30-10:50 Break		15:50-16:10 Break		
	<b>Section 4</b> Chair: Peifeng Su (苏培峰)	10:50- 11:50	<b>Graph neural networks as a general framework for the design and understanding of materials</b> Tian Xie (谢天), MIT	16:10- 18:00	<b>Tutorial: SISSO</b> Tutor: Runhai Ouyang (欧阳润海)
		11:50- 12:20	<b>Automatic Retrosynthetic Pathway Planning Using Template-free Models</b> Kangjie Lin (林康杰), Peking University		<b>Tutorial: CGCNN/GDyNN</b> Tutor: Tian Xie (谢天)
6 <sup>th</sup> Sept.	<b>Section 5</b> Chair: Zexing Cao (曹泽星)	08:30- 09:30	<b>Machine Learning of equivariant functions inspired by atomistic modeling and three-dimensional image processing</b> Bastiaan Braams, Centrum Wiskunde & Informatica, NL	14:00- 15:50	<b>Tutorial: AiiDA</b> Tutors: Leopold Talirz, Jusong Yu (余桔颂), Yunpei Liu (刘云霈), Jingfang Xiong (熊景 放)
		09:30- 10:30	<b>The AiiDA Ecosystem for Computational Materials Science</b> Leopold Talirz, EPFL, Switzerland		
	10:30-10:50 Break		15:50-16:10 Break		
		10:50- 12:20	<b>Tutorial: AiiDA</b> Tutor: Leopold Talirz	16:10- 17:10	<b>Tutorial: AiiDA</b> Tutors: Leopold Talirz, Jusong Yu (余桔颂), Yunpei Liu (刘云霈), Jingfang Xiong (熊景 放)

## 厦门地图



[厦门大学地图](#)



## 厦门交通

厦门机场、火车站(厦门站和厦门北站)到厦大可坐公交车或打的，北站也可选乘地铁到妇幼站再转乘公交车到厦大或选乘 BRT 到眼科医院站再转乘公交车到厦大。乘坐公交车在“**厦大西村**”车站下车离宾馆和注册处最近。

## 入校园证件

第一次进厦大校园请凭从 Workshop 微信群下载的录取通知书。报到注册之后，胸牌可作为进入校园证件。

## 注册

9月3日14:00-20:00在卢嘉锡楼大厅。晚到的学员请于9月4日早上8:00在化学报告厅门口补注册。

## 教室

每天上午报告地点在化学报告厅，下午tutorial地点在同安二106。

## 胸牌

请学员们听报告、参加tutorial时务必佩戴胸牌，凭胸牌入场。主讲人佩戴蓝色胸牌，学员佩戴绿色胸牌，工作人员及志愿者佩戴紫色胸牌。

## 无线网络

我校已加入全球教育机构 eduroam 无线网漫游联盟，学员在学校中搜寻到 eduroam 无线信号后，可以使用原 eduroam 账号密码登录使用；在化学楼卢嘉锡楼一定范围内，可以连接 Chem-Free 使用无线网络，化学报告厅可以连接 meeting 使用无线网络，均无需密码。

## 晚宴

晚宴安排在 9 月 6 日晚上 17:45，地点在艾尼壹水湾。统一安排接送，9 月 6 日下午 17:15 在群贤校门上车。

## 住宿

格林豪泰（演武路下沃仔 13 号）。厦大西校门斜对面光大银行和豪客来中间的路口进去，前行 60 米左转（演武花园对面小巷子进去）。电话 0592-2353333，范先生：18774412275。

## 游泳

特别注意：禁止到海里游泳，陌生海域和潮水起落十分危险。如有意外，后果自负。

## 联系方式

电话：郑老师 15759585212/曹老师 18959283096

邮箱：[pcoss-skl@xmu.edu.cn](mailto:pcoss-skl@xmu.edu.cn)

## Advances in interatomic potentials for materials

Gábor Csányi

*Department of Engineering, University of Cambridge*

Modelling the atomic scale properties of materials is one of the success stories of materials modelling over the past four decades. Increasingly complex functional forms, from pair potentials to embedded atom models and bond order potentials, allowed the quantitative description of different crystal structures, point and line defects, surfaces, shedding light on many elementary processes governing failure, phase stability, etc. Interestingly, the accuracy with which these models describe the potential energy surface corresponding to the electronic ground state has not changed over the decades and is rather limited. The success is thus largely empirical in nature - and follows from the sophistication of the modeller and the judicious compromises made in order to solve specific problems. The parallel developments in electronic structure theory on the other hand provided exquisite quantitative agreement with experiments e.g. for thermomechanical properties, phase stability, and defect energetics. I will report on recent work of a growing community, who have managed to bring these two worlds together, and construct extremely accurate functional representations of the interatomic potential. These developments rely on a very large amount of highly accurate electronic structure data, on non-parametric function fitting, and on sophisticated representation theory that brings with it guarantees of completeness and convergence.

**Bio:** Gábor Csányi got his PhD in computational physics, Massachusetts Institute of Technology 2001. He became Professor of Molecular Modelling in Department of Engineering at Cambridge in 2016. He is an expert in atomistic simulation, particularly in multi scale modelling that couples quantum mechanics to larger length scales. He is currently engaged in applying machine learning techniques to materials modelling problems e.g. deriving force fields (interatomic potentials) from ab initio data. He is also interested in statistical problems in molecular dynamics, e.g. in enhanced sampling algorithms that can be used to automate the calculation of phase diagrams from atomistic models. Some of the modelling work may have applications in robust optimization, and also in understanding materials failure.

# Global Neural Network Potential from Construction to Simulation

Zhipan Liu

*Department of Chemistry, Fudan University, Shanghai, China;  
E-mail: zpliu@fudan.edu.cn*

While the underlying potential energy surface (PES) determines the structure and other properties of material, it has been frustrated to predict new materials from theory even with the advent of supercomputing facilities. The accuracy of PES and the efficiency of PES sampling are two major bottlenecks, not least because of the great complexity of material PES. This lecture introduces a “Global-to-Global” approach for material discovery by combining for the first time the global optimization method with neural network (NN) techniques. The novel global optimization method, the stochastic surface walking (SSW) method is carried out massively in parallel for generating a global training data set, the fitting of which by the atom-centered NN produces a multi-dimensional global PES; the subsequent SSW exploration of large systems with the analytic NN PES can provide key information on the thermodynamics and kinetics stability of unknown phases identified from global PES. We describe in detail the current implementation of the SSW-NN method with particular focuses on the size of the global data set and the simultaneous energy/force/stress NN training procedure. All these methods have been implemented in LASP software ([www.lasphub.com](http://www.lasphub.com)). A number of important functional materials, in particular those for catalysis e.g. ZnCrO oxides, are utilized as the examples to demonstrate the automated global data set generation, the improved NN training procedure and the application in material discovery and catalysis. As a general tool for material simulation, the SSW-NN method provides an efficient and predictive platform for large-scale computational material screening.

## References

- [1] S. D. Huang, C. Shang\*, P. L. Kang, X. J. Zhang and Z. P. Liu\*, WIREs Comput Mol Sci. (2019) e1415. <https://doi.org/10.1002/wcms.1415>
- [2] S. D. Huang, C. Shang, P. L. Kang and Z. P. Liu\*, Chem. Sci. (2018) 9, 8644
- [3] S. D. Huang, C. Shang, P. L. Kang, X. J. Zhang and Z. P. Liu\*, Chem. Sci. (2017) 8, 6327
- [4] S. Ma, S. D. Huang, Z. P. Liu\*, Nature Catalysis (2019) DOI: 10.1038/s41929-019-0293-8

**Bio:** Zhipan Liu got Ph.D in 2003 from Queens Univ Belfast under supervision of Prof. Peijun Hu, and then did PostDoc with Professor David King in University of Cambridge. He returned to China in 2005 and is now a full professor in Department of Chemistry, Fudan University. He has published more than 150 research papers, including 24 in JACS. He was appointed as Senior Editor for J. Phys. Chem. A/B/C since 2017. Zhipan Liu’s research focuses on the reactivity prediction of chemical systems for energy storage and conversion. Novel theoretical methods, such as the stochastic surface walking global optimization (SSW) method and more recently global neural network method, were developed in the group to search for novel structures of material and to identify low energy pathways.

# **Ab initio thermodynamics with the help of machine learning**

Bingqing Cheng

*Trinity College, the University of Cambridge*

A central goal of computational physics and chemistry is to predict material properties using first principles methods based on the fundamental laws of quantum mechanics. However, the high computational costs of these methods typically prevent rigorous predictions of macroscopic quantities at finite temperatures, such as heat capacity, density, and chemical potential.

In this talk, I will discuss how to enable such predictions by combining advanced free energy methods with data-driven machine learning interatomic potentials. I will show that, for the omnipresent and technologically essential system of water, a first-principles thermodynamic description not only leads to excellent agreement with experiments, but also reveals the crucial role of nuclear quantum fluctuations in modulating the thermodynamic stabilities of different phases of water.

## **References**

- [1] B. Cheng, J. Behler, M. Ceriotti, Journal of Physical Chemistry Letters 7 (2016) 2210-2215.
- [2] B. Cheng, M. Ceriotti, Physical Review B 97 (2018) 054102.
- [3] B. Cheng, E. A. Engel, J. Behler, C. Dellago, M. Ceriotti, Proceedings of the National Academy of Sciences 116 (2019) 1110-1115.

**Bio:** Bingqing Cheng works as a junior research fellow at Trinity College, the University of Cambridge. She did undergrad and Master's degrees in Shanghai Jiao Tong University and the University of Hong Kong, and obtained a PhD in Materials Science from Ecole Polytechnique Fédérale de Lausanne, Switzerland. Bingqing's research involves using computer simulations to understand and predict material properties, with a particular focus on exploiting machine-learning methods to extend the scope of atomistic simulations.

# Integrating Machine Learning and Molecular Modelling for Drug Design

Jianing Lu

*Department of Chemistry, New York University*

Structure-based drug design is critically dependent on accuracy of molecular docking scoring functions, and there is of significant interest to advance scoring functions with machine learning approaches. In our current work, by judiciously expanding the training set, exploring new features related to explicit mediating water molecules as well as ligand conformation stability, and apply extreme gradient boosting (XGBoost) with  $\Delta$ -Vina parameterization, we have improved robustness and applicability of machine-learning scoring functions. The new scoring function  $\Delta_{\text{vina}}\text{XGB}$  can not only perform consistently among the top compared to classical scoring functions for the CASF-2016 benchmark, but also achieves significantly better prediction accuracy in different types of structures that mimic real docking applications. Ligand conformation stability plays very important role in  $\Delta_{\text{vina}}\text{XGB}$  scoring function development. However, currently computational estimation of ligand conformation stability is mostly dependent on molecular mechanical force fields, which is computationally efficient but is limited by the accuracy of force fields. Therefore, we explored how machine learning can be used to predict molecular atomization energies and conformation stability using optimized geometries from Merck Molecular Force Field (MMFF). Based on the recently introduced deep tensor neural network (DTNN) approach, we demonstrated importance of training efficiency improvement, hyper-parameter search as well as data augmentation in the optimization of machine learning models, and developed a DTNN\_7ib model which has a much-improved test accuracy. Then using atomic vector representations in the DTNN\_7ib model, we employed transfer learning strategy to train read-out layers and two MMFF-based models have been developed. Our results indicate that DFT-level accuracy of molecular energy prediction can be achieved using force-field optimized geometries and atomic vector representations learned from deep tensor neural network, and integrated molecular modeling and machine learning would be a promising approach to develop more powerful computational tools for molecular conformation analysis.

**Bio:** Jianing Lu graduated from Xiamen University in 2015 with a Bachelor of Science in Chemistry. Her undergraduate research with Prof. Zexing Cao focused on molecular modelling of bio-system. After graduation, she joined Prof. Yingkai Zhang's lab in New York University. She is interested in integrating machine learning methods and molecular modelling to develop powerful tools for drug design.

# Deep Learning for Multi-Scale Molecular Modeling

Linfeng Zhang

*Program in Applied and Computational Mathematics, Princeton University, Princeton,  
New Jersey 08544, USA  
Email: linfengz@princeton.edu*

Deep learning has emerged as a promising tool for a variety of applications in scientific modeling. However, constructing reliable and practical deep learning-based physical models is still a very non-trivial task. In this talk, we discuss the important issues and illustrate the relevant ideas in the context of constructing potential energy and free energy surfaces for molecular modeling. In particular, we will discuss the Deep Potential and Deep Potential Generator scheme for boosting ab-initio molecular dynamics and the Reinforced Dynamics for enhanced sampling and free energy calculation. Extensions to some electronic information and applications to the phase diagram and dielectric properties of reactive water, the warm dense matter systems, as well as many-component alloy and battery systems, etc., will be presented at the end of this talk.

**Bio:** Linfeng Zhang graduated from Peking University in 2016. He is now a graduate student in the Program in Applied and Computational Mathematics (PACM), Princeton University, working with Profs. Roberto Car and Weinan E. Linfeng is interested in various mathematical problems originated from different disciplines of science. Most recently he has been focusing on developing deep learning based models for quantum chemistry, molecular dynamics, as well as enhanced sampling. Linfeng is one of the main developers of DeePMD-kit, a very popular deep learning based open-source software for molecular dynamics.

# Data-Driven Materials Discovery with the Method SISSO

Runhai Ouyang

*The Materials Genome Institute, Shanghai University*

The Materials-Genome Initiative has fostered high-throughput calculations and experiments, leading to large amount of materials data available in literature and databases. Analyzing those data and finding physical descriptors that describe and predict the target materials properties and functions is crucial for knowledge-guided low-cost and fast material discovery. In this regard, efficient data-driven approaches for descriptor identification are required, and many methods falling under the umbrella name of (big-) data analytics (e.g. data mining, machine learning, compressed sensing, etc.) have been developed and applied to the wealth of Materials Science data. In this talk, Ouyang will introduce the recent data-driven method SISSO, which is based on the theory of compressed sensing, for identifying low-dimensional descriptors (A descriptor is defined as a set of features that capture the underlying mechanisms of the target materials property or function; the dimension is the number of features in the descriptor) from huge feature spaces. He will review several recent applications of SISSO across Materials Science and Chemistry for materials discovery: materials map for predicting 2D and 3D topological insulators; new tolerance factor for predicting the stability of perovskite; descriptor for predicting the pressure-induced insulator→metal transition of binary crystals; model for predicting the Gibbs free energy of crystalline solids; and the functional form for predicting superconducting critical temperature. In addition, he will also introduce the newly developed technique in SISSO for multi-task learning for finding a common descriptor for multiple materials properties.

(The SISSO code is freely available at <https://github.com/rouyang2017/SISSO>, and tutorials can be found at <https://analytics-toolkit.nomad-coe.eu/home/> )

**Bio:** Runhai Ouyang joined Shanghai University, China, in 2019 as an associate professor at the Materials Genome Institute. He obtained his PhD degree in physical chemistry in 2014 (advisor: Prof. Wei-Xue Li) from the Dalian Institute of Chemical Physics, Chinese Academy of Sciences. After one year at The University of Sydney and one year at the University of California Riverside for postdoctoral research, he joined the Theory department of Fritz Haber Institute of the Max Planck Society in Berlin and worked with Luca M Ghiringhelli and Matthias Scheffler for the NOMAD project for three years with the research topic data-driven materials science. In collaboration with Ghiringhelli, Scheffler, Curtarolo and Ahmetcik, he created the compressed-sensing method SISSO (sure independence screening and sparsifying operator) for data-driven materials discovery.

# **Graph neural networks as a general framework for the design and understanding of materials**

Tian Xie

*Department of Materials Science and Engineering, MIT*

The exponential increase of open materials data in the past few years poses a challenge to the community to efficiently utilize them for designing better materials. In this talk, I will present our recent works showcasing how graph neural networks can be used as a general framework to utilize large quantities of material data. We will first define the key architecture of crystal graph convolutional neural networks (CGCNN) to represent an arbitrary atomic structure. Then, we will demonstrate how to achieve state-of-the-art performance in predicting material properties and extract material design knowledge from the networks using this framework. Further, we will show several examples of applying this approach to the design of lithium-ion batteries. Finally, we will present our latest work that extends this approach to learn from molecular dynamics simulation trajectories without supervision and understand lithium-ion transport mechanism.

**Bio:** Tian Xie is a PhD student from the department of materials science and engineering at Massachusetts Institute of Technology, advised by Prof. Jeffrey Grossman. He received a B.S. in chemistry from Peking University in 2015. In 2019, he was a PhD software intern at X (formerly Google X), working on an early stage project combining machine learning and physics. After that, he joined DeepMind as a research intern. Tian's research focuses on the development of machine learning algorithms for materials design, and he works closely with several groups from MIT and CMU to apply those algorithms to the discovery of materials for energy innovations. He developed CGCNN (Crystal Graph Convolutional Neural Networks) as a general approach to represent materials in 2017.

# Automatic Retrosynthetic Pathway Planning Using Template-free Models

Kangjie LIN

*BNLMS, State Key Laboratory for Structural Chemistry of Unstable & Stable Species,  
College of Chemistry & Molecular Engineering, Peking University, Beijing, 100871,  
PR China*

Retrosynthetic route planning can be considered a rule-based reasoning procedure. The possibilities for each transformation are generated based on collected reaction rules, and then potential reaction routes are recommended by various optimization algorithms. Although there has been much progress in computer-assisted retrosynthetic route planning and reaction prediction, fully data-driven automatic retrosynthetic route planning remains challenging. Here we present a template-free approach that is independent of any reaction template, rules, or atom mapping, to implement automatic retrosynthetic route planning. We treated each reaction prediction task as a data-driven sequence-to-sequence problem using the multi-head attention-based Transformer architecture, which has demonstrated power in machine translation tasks. Using reactions from United States patent literature, our end-to-end models naturally incorporate the global chemical environments of molecules and achieve state-of-the-art performance on top-1 predictive accuracy (63.0%) and top-1 molecular validity (99.6%) in one-step retrosynthetic tasks. Inspired by the success rate of the one-step reaction prediction, we further carried out iterative, multi-step retrosynthetic route planning for four case products, which was successful. We then constructed an automatic data-driven end-to-end retrosynthetic route planning system (AutoSynRoute) using Monte Carlo Tree Search with a heuristic scoring function. AutoSynRoute successfully reproduced published synthesis routes for the four case products. The end-to-end model for reaction task prediction can be easily extended to larger or customer-requested reaction databases. Our study presents an important step in realizing automatic retrosynthetic route planning.

**Bio:** Kangjie Lin is pursuing his PhD degree in computational chemistry in Peking University (2017~) under the supervision of Professor Luhua Lai. He is currently engaged in applying machine learning techniques to computer-aided synthesis planning and molecular property prediction. He is also interested in de novo molecule design and automated synthesis of chemicals.

# Machine Learning of equivariant functions inspired by atomistic modeling and three-dimensional image processing

Bastiaan Braams

*Centrum Wiskunde & Informatica (CWI), Amsterdam and Dalian Institute of Chemical Physics (DICP), Dalian*

In my talk I noted several works that use (finally) linear regression: the Gaussian Approximation Potential (Gábor Csányi et al.), Solid Harmonic Wavelet Scattering (Stéphane Mallat et al.) and the Atomic Cluster Expansion (Ralf Drautz). I also described recent work employing deep neural networks and there I emphasized two key aspects of the some of the recent work: the networks are structured and parameterized.

Structured: Relative to a standard feed-forward neural network, in these networks each "neuron" holds a structured value and the layer-to-layer connections are compatible with that structure. The concept is familiar from machine vision where the structured value is a two-dimensional array of real values (a pixel image in the input layer) and the compatible operation is a convolution with compact kernel. In our applications the structured value can be a feature vector (in the SchNet approach from Berlin) or also an object that has well-defined transformation properties under rotations of 3D space (in the equivariant neural networks from the Amsterdam group, the Tensor Field networks from the Google people and the more recent DeepPot work from Princeton).

**Bio:** Bastiaan braams is an affiliated researcher in the Multiscale Dynamics group in DICP (December 2016 - present). Previously employed at International Atomic Energy Agency (IAEA), Vienna, Austria (2009-2016), Emory University, Atlanta, GA (2003-2009), New York University, New York City, NY (1989-2003), Princeton Plasma Physics Laboratory, Princeton, NJ (1986-1989) and on PhD research at FOM Institute for Plasma Physics (now DIFFER), Nieuwegein, Netherlands. The PhD work was done at Max Planck Institute for Plasma Physics, Garching, Germany and at UKAEA Culham Laboratory. Basic university education in Utrecht (theoretical physics) and Eindhoven (mathematics and computing science). Interested in scientific computing and data analysis with applications in plasma physics, molecular modelling, and atomic physics. His has a broad view of research interest, including fusion energy research, quantum chemistry and molecular modelling.

# The AiiDA Ecosystem for Computational Materials Science

Leopold Talirz

*EPFL, Switzerland  
Email: leopold.talirz@epfl.ch*

AiiDA ([aiida.net](http://aiida.net), [1]) is a workflow manager for computational science with a strong focus on provenance, performance and extensibility. When executing a workflow, AiiDA records the provenance – calculations performed, codes used and data generated – in a directed acyclic graph tailored to provide full reproducibility of any given result. The AiiDA engine relies on a message queue in order to support high-throughput use cases of up to 50k calculations per hour, and the relational database backend enables performant queries on graphs of millions of nodes. AiiDA plugins extend the core python framework in numerous ways, from new workflows and connections to new simulation codes, support for alternative job schedulers, transport protocols or extensions of the AiiDA command line interface. While domain experts may install AiiDA on their own hardware, the AiiDA lab web platform gives novice users access to their personal AiiDA environment in the cloud, where they can run and manage workflows through tailored and lightweight web applications in the browser. The ecosystem is completed by the Materials Cloud dissemination portal ([materialscloud.org](http://materialscloud.org)), where researchers can publish their AiiDA graphs, thus providing access not only to the results of calculations, but to every step along the way. Peers can browse the database interactively, download individual files or the whole database, and start their research right from where the original author left off.

## References

- [1] Pizzi, G. et al. Comp. Mat. Sci. (2016) 111, 218–230. [10.1016/j.commatsci.2015.09.013](https://doi.org/10.1016/j.commatsci.2015.09.013).

**Bio:** Leopold Talirz got his PhD in Hutter group, University of Zurich in 2015. He was rewarded Empa Research Award for Ph.D. thesis and then he got SNF Early Postdoc. Mobility Fellow, Godby group, University of York, England, working on implemented many-body perturbation theory approximations in model code to compare against exact solutions of the Schrödinger equation. Since 2017, he worked as Postdoc in THEOS and LSMO groups, EPF Lausanne, Switzerland. Now he is endeavor to develop the Materials Cloud open science platform and the AiiDA framework for high-throughput calculations and provenance tracking, and adapting them for the study of nanoporous materials.

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