Haoran Ni

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🌐 haoran-ni.github.io
 haoran-ni
 Haoran Ni

Education

2023 – 2027	**Carnegie Mellon University**	*Pittsburgh, United States*
	Ph.D. in Materials Science	
Advisor	Prof. Noa Marom	
Research	Computational materials modeling, Molecular interfaces, Density functional theory, Machine learning interatomic potentials	
2020 – 2022	**École Polytechnique Fédérale de Lausanne (EPFL)**	*Lausanne, Switzerland*
	Master of Science in Physics	
Advisor	Prof. Michele Ceriotti	
Research	Machine learning interatomic potentials	
2016 – 2020	**Lanzhou University**	*Lanzhou, China*
	Bachelor of Science in Physics (*Honorary Degree*)	
Advisor	Prof. Xiaolong Fan	
Research	Spintronics	
GPA	4.11; Ranked the 4th out of 227 students in Physics; **Top 2%**	

Publications

Structure prediction of organic/inorganic interfaces with Genarris Interfaces

Haoran Ni[†], Kevin Larkin[†], Wen Wen, Saeed Moayedpour, Rithwik Tom, Imanuel Bier, Derek Dardzinski, Noa Marom

In preparation

Open Molecular Crystals 2025 (OMC25) Dataset and Models

Vahe Gharakhanyan, Luis Barroso-Luque, Yi Yang, Muhammed Shuaibi, Kyle Michel, Daniel S. Levine, Misko Dzamba, Xiang Fu, Meng Gao, Xingyu Liu, **Haoran Ni**, Keian Noori, Brandon M. Wood, Matt Uyttendaele, Arman Boromand, C. Lawrence Zitnick, Noa Marom, Zachary W. Ulissi, Anuroop Sriram

arXiv preprint arXiv:2508.02651 (2025)

Physics-inspired equivariant descriptors of nonbonded interactions

Kevin K. Huguenin-Dumittan[†], Philip Loche[†], **Haoran Ni**, Michele Ceriotti

The Journal of Physical Chemistry Letters, 14(43), 9612-9618 (2023)

Observation of spin-orbit magnetoresistance in CoFeB/heavy metal/MgO with existence of both spin Hall effect and Edelstein effect

Haoran Ni, Shuangfeng Li, Qihan Zhang, Jiguang Yao, Yongwei Cui, Xiaolong Fan, Desheng Xue

arXiv preprint arXiv:1909.12811 (2019)

Equal contributions are denoted using †.

Awards

2025	**Richard King Mellon Foundation Presidential Fellowship in Energy**	
2020	**Hong Kong PhD Fellowship Scheme (HKPFS)**	*Declined*
2020	Excellent Graduation Thesis at Lanzhou University	
2018	National English Competition for College Students	*Grand Prize*
2018	The Scientific Research and Innovation Scholarship	*First Prize*
2018	Excellent Student Scholarship at Lanzhou University	*Third Prize*
2018	Outstanding Student of Lanzhou University	
2017	**National Scholarship**	
2017	National English Speech Competition for College Students	*Bronze Medal*
2015	**Chinese Mathematical Olympiad**	*First Prize in Jiangsu Province*
2015	**Chinese Chemistry Olympiad**	*First Prize in Jiangsu Province*

Teaching

2025 Spring   Quantum Mechanics of Materials - 27710
Grading, Teaching, Recitation

Standarized Tests

Oct. 2022   **TOEFL** (110)

- Reading: 30/30
- Listening: 26/30
- Speaking: 25/30
- Writing: 29/30

Oct. 2022   **GRE General** (331 + 4.0)

- Verbal Reasoning: 161/170
- Quantitative Reasoning: 170/170
- Analytical Writing: 4.0/6.0

Skills

Programming	Python, Shell, LaTeX, pine script	Packages	PyTorch, SciPy, NumPy, ASE, pymatgen, Transformers, LangChain
DFT	FHI-aims, VASP	OS	Linux, MacOS, Windows
HPC	Slurm, mpi4py		

Leadership & Arts

2023 – 2024   CMU Chinese Students & Scholars Association
Executive Board

2020 – 2022   EPFL Chinese Students & Scholars Association
Vice President

2020 – Now   NetEase Cloud Music Artist
Amateur Musician

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⚉ Haoran Ni

教育经历

2023 – 2027	**卡内基梅隆大学（CMU）**	**材料科学博士**
导师	Prof. Noa Marom	
研究方向	计算材料，分子界面，密度泛函计算，机器学习原子势	

2020 – 2022	**洛桑联邦理工学院（EPFL）**	**物理学硕士**
导师	Prof. Michele Ceriotti	
研究方向	机器学习原子势	

2016 – 2020	**兰州大学**	**理学学士（物理学）**
导师	范小龙教授	（萃英学院荣誉学位)
研究方向	自旋电子学	
学分绩	4.11; 院系排名 4/227; **前 2%**	

论文发表

Structure prediction of organic/inorganic interfaces with Genarris Interfaces

Haoran Ni[†], Kevin Larkin[†], Wen Wen, Saeed Moayedpour, Rithwik Tom, Imanuel Bier, Derek Dardzinski, Noa Marom

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Haoran Ni, Shuangfeng Li, Qihan Zhang, Jiguang Yao, Yongwei Cui, Xiaolong Fan, Desheng Xue

arXiv preprint arXiv:1909.12811 (2019)

† 标注共同一作.

获奖经历

2025	**Richard King Mellon Foundation Presidential Fellowship**	共 89,560 美元
2020	**香港政府奖学金（HKPFS）**	已回拒
2020	兰州大学优秀毕业论文	
2018	全国大学生英语竞赛	特等奖（省第六名）
2018	兰州大学科研创新奖学金	一等奖
2018	兰州大学优秀学生奖学金	三等奖
2018	兰州大学学生标兵	
2017	**国家奖学金**	
2017	全国大学生英语演讲比赛	全国铜牌
2017	全国大学生英语竞赛	特等奖（省第二名）
2015	**全国高中生数学联赛**	江苏省一等奖
2015	**全国高中生化学奥林匹克竞赛**	江苏省一等奖

教学经历

2025 春季学期　Quantum Mechanics of Materials - CMU 27710

作业批改, 代课, 习题课

标化考试

2022　**托福（TOEFL）**（总分：110）
- 阅读: 30/30
- 听力: 26/30
- 口语: 25/30
- 写作: 29/30

2022　**GRE General**（总分：331 + 4.0）
- 阅读: 161/170
- 数学: 170/170
- 写作: 4.0/6.0

2017　**英语六级**（总分：601）

2016　**英语四级**（总分：634）

技能

编程语言	Python, Shell, LaTeX, pine script	编程包	PyTorch, SciPy, NumPy, ASE, pymatgen, Transformers, LangChain
第一性计算	FHI-aims, VASP	操作系统	Linux, MacOS, Windows
高性能计算	Slurm, mpi4py		

课外活动

2023 – 2024　卡内基梅隆大学中国学生学者联合会（CMU CSSA）
　　　　　　　执行主席团

2020 – 2022　洛桑联邦理工学院中国学生学者联合会（EPFL CSSA）
　　　　　　　副主席

2020 – Now　网易云音乐
　　　　　　　网易音乐人