Han Yang, Ph.D.

Senior Researcher at Microsoft

+86-13222009007
yanghan234@outlook.com

Summary

Han is a highly skilled computational researcher with a strong background in quantum chemistry, physics, mathematics, and scientific computing. With a focus on first-principles numerical simulations and high-performance computing, Han is dedicated to developing innovative predictive methods that accelerate the discovery of novel materials. To learn more about Han's work and achievements, please visit my personal page: https://yanghan.dev

Education

- **Ph.D. in Chemistry (Computational)**, *The University of Chicago*, Chicago, Illinois
  Sept. 2016 – Dec. 2021
  Dissertation: *Electron-Electron and Electron-Phonon Interactions in Semiconductors and Insulators from Many-Body Perturbation Theory.*
- **Master of Science in Chemistry**, *The University of Chicago*, Chicago, Illinois
  Sept. 2016 – Dec. 2017
- **Bachelor of Science in Chemistry**, *Nanjing University*, Nanjing, Jiangsu, China
  Sept. 2012 – Jun. 2016

Research Experience

- **Senior Researcher**, *Microsoft Research AI4Science*, Shanghai, China
  Aug. 2022 – Current
  - Conducted high-throughput investigation of thermal conductivity of materials using deep learning techniques, resulting in a forthcoming publication and patent application.
  - Executed high-throughput calculation of millions of materials using Density Functional Theory (DFT) in VASP. Devised a streamlined and resilient workflow on Microsoft Azure's cloud computing platform, demonstrating exceptional technical expertise and substantially improving the screening process.
  - Accelerated quantum chemistry calculations by $\mathbf{5-10x}$ using CUDA on Nvidia GPUs, demonstrating expertise in advanced computational methods.

- Played a key role in advancing deep learning models for incorporating long-range interactions and deriving a formalism that validated our developments, which leads to a **40% reduction in error** compared to existing methods.
- Contributed to the development of a machine-learned force field (ML-FF), performing post-processing tasks, and employing **active learning** strategy to enhance and supplement the data set, showcasing strong analytical abilities and technical expertise.

- **Research Assistant**, *The University of Chicago*, Chicago, Illinois, US
  Sept. 2016 – Dec. 2021
  - Solid knowledge of Density Functional Theory (DFT), Density Functional Perturbation Theory (DFPT) and Many-body Perturbation Theory (MBPT).
  - First-hand experience with DFT calculations using `Quantum Espresso`, ab initio molecular dynamics (AIMD) using `Qbox` code and G_0W_0 calculations using `WEST` code.
  - Extensive experience with parallel computing using Message Passing Interface (MPI); Extensive experience running high performance computation on supercomputers.
  - 5 years experience with Linux programming environment, and Fortran, C++ programming languages.
  - Implemented massively parallelized Fortran codes on supercomputers to compute electron-phonon interactions in large scale materials.
  - Carried out simulations on world-leading supercomputers, including Mira (Argonne National Laboratory) and Cori (National Energy Research Scientific Computing Center).
  - Extensive experience using Python, Jupyter Notebook and Python libraries including Numpy, Pandas, Matplotlib and Flask.
- **Undergraduate Researcher**, *Nanjing University*, Nanjing, Jiangsu, China
  Sept. 2014 – Jun. 2016
  - Developed and implemented a framework to reduced the computational cost of excitation energies in molecules.

Teaching Experience

- **Teaching Assistant**, *Comprehensive General Chemistry*, Chicago, Illinois
  Spring Quarter, 2018
- **Teaching Assistant**, *Collaborative Learning in General Chemistry*, Chicago, Illinois
  Winter Quarter, 2017
- **Teaching Assistant**, *Collaborative Learning in General Chemistry*, Chicago, Illinois
  Autumn Quarter, 2016

Publications

- Yunyang Li, Yusong Wang, Lin Huang, **Han Yang**, Xinran Wei, Jia Zhang, Zun Wang, Tong Wang, Bin Shao, Tie-Yan Liu. Long-Short-Range Message-Passing: A Physics-Informed Framework to Capture Non-Local Interaction for Scalable Molecular Dynamics Simulation. 2023 [link]
- **Han Yang**, Marco Govoni, Arpan Kundu, Giulia Galli. Computational Protocol to Evaluate Electron-Phonon Interactions within Density Matrix Perturbation Theory. J. Chem. Theory Comput. 18 (10), 6031–6042, 2022 [link]
- **Han Yang**. Electron-Electron and Electron-Phonon Interactions in Semiconductors and Insulators from Many-Body Perturbation Theory. Ph.D. Dissertation, The University of Chicago, 2021 [link]
- **Han Yang**, Marco Govoni, Arpan Kundu, Giulia Galli. Combined First-Principles Calculations of Electron–Electron and Electron–Phonon Self-Energies in Condensed Systems. J. Chem. Theory Comput. 17 (12), 7468-7476, 2021 [link]
- Arpan Kundu, Marco Govoni, **Han Yang**, Michele Ceriotti, Francois Gygi, Giulia Galli. Quantum Vibronic Effects on the Electronic Properties of Solid and Molecular Carbon. Phys. Rev. Materials 5 (7), L070801, 2021 [link]
- **Han Yang**, Marco Govoni, Giulia Galli. Improving the Efficiency of G_0W_0 Calculations with Approximate Spectral Decompositions of Dielectric Matrices. J. Chem. Phys. 151 (22), 224102, 2019 [link]

Talks

- Electron-Phonon Interactionin Molecules and Solids Using Hybrid Functionals. Contributed talk, American Physics Society March Meeting, Chicago IL & Online (2022)
- Implementation, validation and applications of electron-phonon calculations to large systems. Contributed talk, American Physics Society March Meeting, Online (2021)
- Coupling many-body-perturbation-theory calculations of electron-electron and electron-phonon coupling. Contributed talk, American Physics Society March Meeting, Denver CO (2020)
- Effect of Electron-Phonon Interaction on the Opto-Electronic Properties of Semiconducting Nanoparticles. American Physics Society March Meeting, Boston MA (2019)
- Approximate spectral decomposition of density-density response functions. Contributed talk, American Physics Society March Meeting, Los Angeles CA (2018)

Supervision

- Yiwei Liu, Ph.D. candidate at East China Normal University and intern student at Microsoft
- Zekun Chen, Ph.D. candidate at Univeristy of California, Davis and intern student at Microsoft (co-supervised)

Skills

- **Quantum Chemistry Codes**
  Quantum Espresso, VASP, PySCF
- **Programming Languages:**
  Fortran, Python, C/C++
- **Computing**
  Message Passing Interface (MPI), CUDA, Microsoft Azure Cloud Computing
- **Other Tools**
  Git, Vim, Jupyter Notebook, Pandas, Numpy, Scikit-Learn, Matplotlib, Flask

Languages

Mandarin	Native Speaker
English	Fluent