Yiqun Luo

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EDUCATION

Carnegie Mellon University, Pittsburgh, PA **Aug. 2022 - May 2027 (expected)**
Ph.D. in Physics
Cumulative QPA: 3.98

Peking University, Beijing, China **Aug. 2018 - July 2022**
Bachelor of Science in Physics (Honorary Degree)
Overall GPA: 3.79/4.0 (24/184)

RESEARCH EXPERIENCE

Department of Material Science and Engineering at Carnegie Mellon University **Sep 2022 – Present**
Research Assistant | Advisor: Professor Noa Marom
Application of Machine Learning to Organic Light-Emitting Materials

- Established a common ground data set PAH101, excited states properties of a list of 101 representative poly-cyclic aromatic hydrocarbon (PAH) focusing on time-consuming and high-precision *GW* calculations, for future research about PAH crystals as light absorber/emitter.
- Based on PAH101, applied Sure-Independence-Screening-and-Sparsifying-Operator (SISSO) to predict high-fidelity excited-state properties with the constraints of limited data and explanability requirement.
- Improved previous gap prediction Graph Neural Network (GNN) models and achieved high precision of molecular gap prediction on OE62, a density functional theory data set on about 62k molecules, by applying active learning.

Department of Physics at Peking University **Apr 2020 – Apr 2022**
Research Assistant | Advisor: Professor Huichao Song
Application of Machine Learning to Relativistic Fluid Dynamics

- Applied a Convolutional Neural Network (CNN) to predict the specific shear viscosity of quark gluon-plasma from the measurement of final state particles in heavy-ion collisions with high fidelity and used gradient-weighted class activation mapping, a deep learning algorithm, to visualize the predicted physical pattern.

Department of Physics and Astronomy at University of Minnesota, Twin Cities **July 2021 – Sep 2021**
Research assistant | Advisor: Professor Joseph Kapusta
Consistency and Stability Exploration of a Relativistic Hydrodynamics Theory

- Verified the consistency of a novel hydrodynamics theory (BDNK equations) with the relativistic MIS theory and the non-relativistic Navier-Stokes equation in formalism.
- Numerically established and verified the physicality conditions for BDNK equations that traditional first-order relativistic hydrodynamics theories violated.

PUBLICATIONS

- Gao S, Luo Y, Liu X, Marom N. Predicting the excited-state properties of crystalline organic semiconductors using *GW*+BSE and machine learning. ChemRxiv. 2024; doi:10.26434/chemrxiv-2024-c7csx (Co-first-author)
- Gao S, Liu X, Luo Y, Wang X, Zhao K, Chang V, et al. PAH101: A *GW*+BSE Dataset of 101 Polycyclic Aromatic Hydrocarbon (PAH) Molecular Crystals. ChemRxiv. 2024; doi:10.26434/chemrxiv-2024-ms8x6-v2
- PAH101 dataset. DOI: 10.17172/NOMAD/2024.12.05-1

- Wang X, Gao S, Luo Y, Liu X, Tom R, Zhao K, Chang V, Marom N. Computational Discovery of Intermolecular Singlet Fission Materials Using Many-Body Perturbation Theory. The Journal of Physical Chemistry C. 2024 May 1;128(19):7841-64.
- Zhou M, Luo Y, Song H. Applications of machine learning in relativistic heavy ion physics. SCIENTIA SINICA Physica, Mechanica & Astronomica. 2022 Apr 15; 52(5)

PROJECT EXPERIENCE

Challenge Cup at Beijing, China **Nov 2021 – May 2022**

- Applied a Bayesian Neural Network (BNN) model to learn and predict fission yields with uncertainty quantification on a team of two.
- Achieved top 2% at this a top-rated research competition for college students.

SERVICE

Department of Physics at CMU **Dec 2024 - March 2024**

Admission Committee Member

- Reviewed Ph.D. applications, evaluated candidates, and provided recommendations to the department
- Participated in candidate discussions and contributed to admission decisions.

Department of Physics at CMU **Jan 2024 - May 2024**

Teaching Assistant

- Held regular recitations, communicated with students about challenging material in office hours, and graded Physics I for Engineering Students.

SKILLS

Programming skills: Python (PyTorch, TensorFlow, PyTorch Geometric, CUDA, XPU), C/C++, LaTeX, Markdown, MATLAB

Operating Systems: Windows, Linux

Language: English (professional proficiency), Mandarin (native)

HONORS & AWARDS

Honorary Degree (PKU Scholarship) in Physics, School of Physics, Peking University (top 10%) **July 2022**

Wangchenyang-Chengya Scholarship, School of Physics, Peking University (top 10%) **Sep 2021**

First Prize, the Chinese Mathematics Competitions (twice) (top 0.5%) **Nov 2019 & Nov 2020**

First prize of the 33th Chinese Physics Olympiad, China (top 0.3%) **Sep 2017**

First prize of the 32th Chinese High School Mathematics League, China (top 0.3%) **Sep 2016**

RELEVANT COURSEWORK

Mathematics: Advanced Mathematics, Advanced Algebra, Partial Differential Equations, Probability Theory, Statistics, Group Theory

Physics: Thermodynamics and Statistical Physics, Quantum Mechanics, Many-Body Physics, General Relativity, Quantum Field Theory

Computer Science: Introduction to Machine Learning, Introduction to Deep Learning, Data Structures and Algorithms, Introduction to Computer System, Programming Practice