Jusong Yu

Curriculum Vitae

Personal Information

Date of birth:	China | August 26, 1992
Nationality:	Chinese
Languages:	English (Fluent)
	Chinese (Mother tongue)
	German (A2)
Email:	jusong.d.yu@gmail.com
GitHub:	http://github.com/unkcpz

Tech Stacks

Programming	Python, Rust, Julia, C
Dev tools	Docker, Kubernetes
	Git, neovim
	SQLite, HTMX
Operating system	Linux, Mac OS

Education/Job Experiences

2023-Now	Postdoctoral researcher in Computational condensed matter physics, **Paul Scherrer Institut (PSI)**
2021-2023	Postdoctoral researcher in Computational condensed matter physics, **EPFL**
2017-2021	Ph.D. in Physics, **South China University of Technology**
2014-2021	M.Sc in Physics, **Chinese Academy of Science**
2010-2014	B.Sc. in Polymer Science, **Northwestern Polytechnical University**

Projects

(1) Using Bayesian optimization for generating accurate pseudopotential libraries (on-going)

(2) Lead the redesign of the kernel part of scientific workflow engine AiiDA to achieve extreme large-scale throughput, to enable millions of short, small-scale simulations (on-going)

(3) Julia package for solving the atomic Schrödinger equation and pseudizing to generate pseudopotentials for plane-wave DFT. `https://github.com/unkcpz/PseudopotentialGenerator.jl`

(4) Rust crate **rsdos** with Python API bindings for fast, server-less local file datasets management. `https://github.com/unkcpz/rsdos`

(5) Lead and coordinate **AiiDAlab** development (a web tool for complex computational simulation access) **2022-2024** `https://demo.aiidalab.io`

(6) Mentoring a Google Summer of Code student on the AiiDA project regarding the ranking system for the AiiDA plugin registry **May-Sept 2023** `https://summerofcode.withgoogle.com/archive/2023/projects/B9z9tso7`

(7) The MARKETPLACE project (EU Horizon 2020): Contributing to the project and leading the development of T4.9: HPC integration as a service **Sept. 2021-2023**

(8) Author of aiida-sssp-workflow and aiidalab-sssp for solid-state pseudopotential verification **Sept. 2022-2024**

(9) **Libxc.jl**: a Julia binding to the libxc library for exchange-correlation functionals **Sept. 2019**

Selected Talks

Oct. 2024 | **MolSSI Workshop on Julia for Computational Molecular and Materials Science**, *Pittsburgh, PA (USA)*
AiiDA: a DSL, an ecosystem
https://juliamolsim.github.io/molssi_workshop/

March 2024 | **American Physical Society Conference**, *Minneapolis, MN (USA)*
Reproducible workflows for verification and optimization of solid-state pseudopotentials
https://meetings.aps.org/Meeting/MAR24/Session/A60.10

Oct. 2023 | Huawei Thames Summit & European Innovation Star Workshop, *Cambridge, United Kingdom*
Accelerating materials-science research via reproducible simulations with AiiDA and Materials Cloud

Aug. 2022 | **Psi-k Conference 2022**, *SwissTech Convention Center, EPFL, Lausanne (Switzerland)*
Contributed talk: Making complex scientific workflows accessible and shareable with AiiDAlab – pseudopotentials and electronic-structure simulations on demand
https://www.psik2022.net/

Jun. 2022 | **OPTIMADE Workshop at CECAM**, *CECAM, EPFL, Lausanne (Switzerland)*
Presenting on integrating Materials Cloud databases with OPTIMADE
https://www.cecam.org/workshop-details/1120

Peer-reviewed Publications

(1) Matthew L. Evans, ... **Jusong Yu**, et al. "Developments and applications of the OPTIMADE API for materials discovery, design, and data exchange" *Digital Discovery* **2024** DOI:10.1039/D4DD00039K
Contribution: tool development and text writing of "Data provision" section

(2) Bosoni Emanuele, ... **Jusong Yu**, et al. "How to verify the precision of density-functional-theory implementations via reproducible and universal workflows." *Nature Reviews Physics* **2023** DOI:10.1038/s42254-023-00655-3
Contribution: Generated and tested new pseudopotentials used for Quantum ESPRESSO.

(3) Uhrin Martin, Sebastiaan P. Huber, **Jusong Yu**, Nicola Marzari, and Giovanni Pizzi. "Workflows in AiiDA: Engineering of a high-throughput, event-based engine for robust and modular computational workflows." *Computational Materials Science* **2021** DOI:10.1016/j.commatsci.2020.110086
Contribution: Software (asynchronous part), writing – review and editing.

(4) **Jusong Yu**, ..., Xiaobao Yang. "Motif Based High-Throughput Structure Prediction Of Superconducting Monolayer Titanium Boride." *Physical Chemistry Chemical Physics* **2020** DOI:10.1039/D0CP01540G
Contribution: Conceptualization, software, writing – original draft.

Interests and Extracurricular Activities

Swimming, board games, violin, literature.