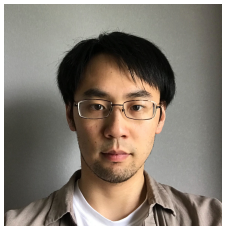

Jusong Yu

Curriculum Vitae

Personal Information

Date of birth:	Zhejiang, 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
Homepage:	https://orange-box.cc/

Tech stacks

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

Projects

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

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

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

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

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

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

(7) The MARKETPLACE project funded by EU Horizon 2020 Contributing to the Project and leading the development of T4.9: HPC integration as a service for the platform **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 Kindom)*
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 **Open Databases Integration for Materials Design (OPTIMADE) workshop at CECAM**, *CECAM, EPFL, Lausanne (Switzerland)*
Presenting on workshop for new development of integrating Materials Cloud databases with OPITMADE
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 developing and text writing of "Data provision" section

(2) Bosoni Emanuele, ... **Jusong Yu**, et al. and Giovanni Pizzi. "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.

Education and job experiences

2023-Now Postdoctoral researcher in Computational Material Science,
Paul Scherrer Institut (PSI)

2021-2023 Postdoctoral researcher in Computational Material Science,
École Polytechnique Fédérale de Lausanne (EPFL)

2017-2021 Ph.D. Studies in Physics,
South China University of Technology

2014-2017 Graduate Studies in Physics,
Chinese Academy of Sciences

2010-2014 Undergraduate Studies in Polymer Science,
Northwestern Polytechnical University,

Interests and Extracurricular Activities

Swimming, Board game, Violin, Literature.