Wei CHEN

Chercheur qualifié
Computational Materials Science

Contact

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11 August 1980

Computing

Languages	Python, Fortran, Bash
HPC	MPI, GPU, Slurm
DevOps	Git, CI/CD, Linux
Data/AI	ML, High-throughput

Languages

English: Fluent
French: A2 (Learning)
Chinese: Native

References

Prof. G.-M. Rignanese
UCLouvain, Belgium

Prof. G. Hautier
Rice University, USA

Prof. A. Pasquarello
EPFL, Switzerland

Professional Experience

IMCN - MODL Pole, UCLouvain, Belgium **2016 – Present**

- **Sustainable energy**: Photocatalysis, high-entropy materials, photovoltaics.
- **Machine learning**: Cluster expansion, MLIPs.
- **Theory developement**: Dielectric dependent hybrid functional.
- **Software Stewardship**: Maintenance of local scientific codebases.

Atomic Scale Simulation, EPFL, Switzerland **2011 – 2016**

- Developed electronic-structure methods (GW, hybrid functionals).
- Implemented vertex corrections for high-accuracy band gap calculations.

Code Developments

- **GCMC**: Grand Canonical Monte Carlo with replica exchange and hybrid MC/MD support for ASE-compatible MLIPs.
- **ABINIT**: XC kernels and vertex corrections; range-separated hybrid functional.
- **Quantum ESPRESSO**: Range-separated hybrid functional implementation.
- **MPEA Stability**: High-throughput alloy prediction webapp.
- **FNV**: Python package for charged defect corrections.

Education

Dr. rer. nat. in Physics (*summa cum laude*) **2011**
Leibniz Universität Hannover, Germany

MSc. in Electrical Engineering **2005**
Fudan University, Shanghai, China

BSc. in Physics **2002**
Fudan University, Shanghai, China

Selected Publications

[1] W. Chen et al., "A map of single-phase high-entropy alloys", Nat. Commun. **14**, 2856 (2023).

[2] W. Chen et al., "Origin of the low conversion efficiency in Cu_2ZnSnS_4 kesterite solar cells: the actual role of cation disorder", Energy Environ. Sci. **14**, 3567 (2021).

[3] W. Chen et al., "High-throughput computational discovery of $In_2Mn_2O_7$ as a high Curie temperature ferromagnetic semiconductor for spintronics", npj Comput. Mater. **5**, 72 (2019).

[4] W. Chen et al., "*Ab initio* electronic structure of liquid water", Phys. Rev. Lett. **117**, 186401 (2016).

[5] W. Chen and A. Pasquarello, "Accurate band gaps of extended systems via efficient vertex corrections in GW", Phys. Rev. B **92**, 041115(R) (2015).