Cong Liu

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School of Physics, Nanjing University, No. 22 Hankou Road, Nanjing 210093, China

Professional experience

Polytechnic University of Catalonia, Spain - physics school postdoctor Sep 2021 - Jan 2022

- Major: Bose-Einstein condensate, Supersolid, Machine-learning potentials (Supervisor: Cazorla Claudio)

Nanjing University, China - physics school Ph.D candidate Aug 2016 - Jun 2021

- Major: Condensed matter physics, Computational physics (Supervisor: Jian Sun)

Huazhong University of Science and Technology, China - physics school B.S. Sep 2012 - Jun 2016

Research interest and experience

I'm mainly interested in the evolution of condensed matter under extreme conditions, such as high pressure and high temperature, by first-principles calculations and (classical or *ab initio*) molecular dynamic simulations.

- Superionic and plastic state under extreme conditions, such as Uranus and Neptune.
- Applications of superionic and plastic phase to enhance the material performance, such as lithium-based battery materials, copper-based thermoelectric materials, and refrigeration agents.
- Melting curve calculations of matter by free energy calculations, two phase coexistence method, Z method, etc.
- Crystal structure predictions with Random Search or Evolution algorithm.
- Materials design with high pressure method, especially high energy density materials, superhard and superconducting materials.

Honors & awards

National scholarship for postgraduates 10/2020

National scholarship for postgraduates 10/2019

Skills

- **Programming skills:** programming with Python, Fortran, C and Linux Shell; picture process with adobe photoshop and adobe illustrator; data crawling or API processing.
- **Computational methods:** first-principle calculations, crystal structure prediction, classical, path integral and ab intio molecular dynamic simulations, etc.
- **Softwares:** VASP, Quantum Espresso, CP2K, Lammps, i-PI, VMD, Phonopy, Material Studio, etc.
- **Interests:** swimming, reasoning game

Publication list

1. **C. Liu**, J. Shi, H. Gao, J. Wang, Y. Han, X. Lu, H.-T. Wang, D. Xing, and J. Sun, *Mixed Coordination Silica at Megabar Pressure,* Phys. Rev. Lett. **126**, 035701 (2021).
2. **C. Liu**, H. Gao, A. Hermann, Y. Wang, MS. Miao, C. J. Pickard, R. J. Needs, H.-T. Wang, D. Xing, and J. Sun, *Plastic and Superionic Helium Ammonia Compounds under High Pressure and High Temperature,* Phys. Rev. X **10**, 021007 (2020).
3. **C. Liu**, H. Gao, Y. Wang, R. J. Needs, C. J. Pickard, J. Sun, H.-T. Wang, and D. Xing, *Multiple Superionic States in Helium-Water Compounds*, Nat. Phys. **15**, 1065 (2019).
4. Y. Wang, J. Wang, A. Hermann, **C. Liu**, H. Gao, E. Tosatti, H.-T. Wang, D. Xing, and J. Sun, *Electronically Driven 1D Cooperative Diffusion in a Simple Cubic Crystal*, Phys. Rev. X **11**, 011006 (2021).
5. H. Gao, **C. Liu**, A. Hermann, R. J. Needs, C. J. Pickard, H.-T. Wang, D. Xing, and J. Sun, *Coexistence of Plastic and Partially Diffusive Phases in a Helium Methane Compound*, Natl. Sci. Rev. **7**, 1540 (2020)
6. K. Xia, J. Yuan, X. Zheng, **C. Liu**, H. Gao, Q. Wu, and J. Sun, *Predictions on High-Power Trivalent Metal Pentazolate Salts*, J. Phys. Chem. Lett. **10**, 6166 (2019).
7. K. Xia, X. Zheng, J. Yuan, **C. Liu**, H. Gao, Q. Wu, and J. Sun, *Pressure-Stabilized High-Energy-Density Alkaline-Earth-Metal Pentazolate Salts,* J. Phys. Chem. C **123**, 10205 (2019).
8. K. Xia, H. Gao, **C. Liu**, J. Yuan, J. Sun, H.-T. Wang, and D. Xing, *A Novel Superhard Tungsten Nitride Predicted by Machine-Learning Accelerated Crystal Structure Search,* Sci. Bull. **63**, 817 (2018).
9. K. Xia, M. Ma, **C. Liu**, H. Gao, Q. Chen, J. He, J. Sun, H.-T. Wang, Y. Tian, and D. Xing, *Superhard and superconducting B6C,* Mater. Today Phys. **3**, 76 (2017).

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