Cong Liu

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Professional experience

Polytechnic University of Catalonia, Spain Sep 2021 - Jan 2022

physics school postdoctor

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

Nanjing University, China Aug 2016 - Jun 2021

physics school Ph.D candidate

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

Huazhong University of Science and Technology, China Sep 2012 - Jun 2016

physics school B.S.

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 Density Functional Theory, Quantum Monte Carlo simulations and Machine-Learning techniques.

- 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.
- Quantum solids, such as Helium-4 and other analogous bosons, toward to the novel supersolid states (a novel quantum state of matter in which both superfluid (or, equivalently, Bose-Einstein condensation) and solid long-range order could coexist).
- 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

Excellent doctoral thesis of Jiangsu Province in 2022, China	12/2022
Margarita Salas Postdoctoral fellowship, Spain	07/2022
National scholarship for postgraduates, China	10/2020
National scholarship for postgraduates, China	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, quantum monte carlo, machine-learning potential, classical, path integral and ab intio molecular dynamic simulations, etc.
- **Softwares:** VASP, Quantum Espresso, DeePMD-kit, CP2K, Lammps, i-PI, VMD, Phonopy, Material Studio, etc.

Publication list

1. **C. Liu**, J. Wang, X. Deng, X. Wang, C. J. Pickard, R. Helled, Z. Wu, H.-T. Wang, D. Xing, and J. Sun, *Partially Diffusive Helium-Silica Compound in the Deep Interiors of Giant Planets,* Chin. Phys. Lett. 39, 076101 (2022).
2. **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).
3. **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).
4. **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).

5. K. Xia, C. Ding, J. Yuan, C. Liu, H. Gao, and J. Sun, *Atomic-Scale Pentagraphene Ribbons Stabilized with Alkali Metals under Moderate Pressures*, Inorg. Chem. 61, 18229 (2022).
6. T. Huang, **C. Liu**, J. Wang, S. Pan, Y. Han, C. J. Pickard, R. Helled, H.-T. Wang, D. Xing, and J. Sun, *Metallic Aluminum Suboxides with Ultrahigh Electrical Conductivity at High Pressure*, Research 2022, (2022).
7. H. Gao, **C. Liu**, J. Shi, S. Pan, T. Huang, X. Lu, H.-T. Wang, D. Xing, and J. Sun, *Superionic Silica-Water and Silica-Hydrogen Compounds in the Deep Interiors of Uranus and Neptune*, Phys. Rev. Lett. 128, 035702 (2022).
8. K. Xia, Q. Chen, H. Gao, X. Feng, J. Yuan, **C. Liu**, S. A. T. Redfern, and J. Sun, *Icosahedral silicon boride: A potential hybrid photovoltaic-thermoelectric for energy harvesting*, Phys. Rev. Materials 5, 115402 (2021).
9. 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).
10. 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)
11. 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).
12. 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).
13. 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).
14. 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).

Reference Email

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Other Link

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