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Quantum Monte Carlo and Machine Learning Calculations for matter under extreme conditions

Dense hydrogen is important because of its ubiquitous presence in the universe, its technological applications and its suitability for developing and testing ab initio simulation methods. Even though it is the "holy grail"of high pressure research, its phase diagram above 100 GPa is uncertain. We have made a new study of its phase diagram using a machine-learned interatomic potential trained with Quantum Monte Carlo (QMC) forces and energies and we find two new stable phases. The high temperature phase has a reentrant melting line with a maximum at higher temperatures (1450K at 150GPa) than previously estimated.

Because continuum QMC methods such as DMC and PIMC are directly formulated in coordinate space, they do not have the limitation of a basis set which helps in disordered systems such as those liquids, chemical reactions, solids with large amplitude motions, and surfaces. Slater-Jastrow-backflow wavefunctions are a compact, efficient and understandable description of systems with strong correlation. An important application for QMC is to provide unbiased data for bespoke force-fields; they have advantages over other accurate electronic structure methods such as those based on DFT. [See Phys. Rev. Lett. 130, 076102 (2023) and arXiv:2310.15994]

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