Exotic new compounds and their states in the interior of giant planets predicted from first-principles calculations

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ABSTRACT

In this talk, I will introduce the methods developed in my group, especially the machine learning and graph theory aided crystal structure prediction method (Magus) [1]. In addition, I will show some applications of these methods combined with first-principles calculations, for instance, the predictions of new possible compounds (helium-water, helium-ammonia, helium-methane, helium-silica, silica-water, etc) in the interior of giant planets or exoplanets, and their exotic new states under planetary high-pressure and high-temperature conditions (superionic state, plastic state, and their coexistence) [2-6]. These new compounds and their states may have some important implications for giant planets, including demixing, magnetic field, erosion of the rocky core, etc.

REFERENCE
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