

Predicted novel helium compounds under high pressure via CALYPSO

Jurong Zhang¹, Xiaolei Feng², Simon A. T. Redfern², Hanyu Liu^{1*}, Changfeng Chen³, Yanming Ma¹

¹Jilin University, 2699 Qianjin Street Changchun 130012, China
²University of Cambridge, Downing Street, Cambridge CB2 3EQ, UK
³University of Nevada, Las Vegas, Nevada 89154, United States

Keywords: high pressure, crystal structure prediction, helium compounds, novel reaction

*e-mail: hanyuliu@jlu.edu.cn

The knowledge of the structures that can exist in compounds containing helium is of interest for understanding the conditions where and if inert element can form stable compounds where closed shell electrons of helium can participate in bonding that is not describable exclusively by van der Waals interactions alone. In this work, we examine some mixtures of He and H₂O, N₂ or some minerals at high pressures using a first-principles structure searching method (CALYPSO). We find some thermodynamically stable structures under pressure[1-3]. These mechanically and dynamically stable structures are found at pressures that are now becoming accessible to high-pressure technique. The present results offer insights for the understanding of the plausible reaction between helium with minerals in the Earth's or other exoplanetary interiors.

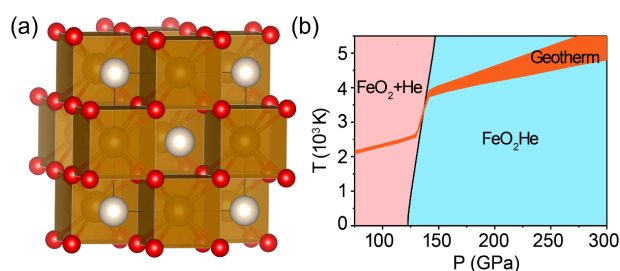


Figure 1. Figure name

Fig. 1 (a) The structure of FeO₂He (b) the P-T phase of FeO₂He.

[1] Yinwei Li, Xiaolei Feng, Hanyu Liu, Jian Hao, Simon A.T. Redfern, Weiwei Lei, Dan Liu, Yanming Ma, *Nature Commun.* 2018, **9**, 722

[2] Jurong Zhang, Jian Lv, Hefei Li, Xiaolei Feng, Simon A.T. Redfern, Cheng Lu, Hanyu Liu, Changfeng Chen, Yanming Ma, *Phys. Rev. Lett.* 2018, **121**, 255703

[3] Hanyu Liu, Yansun Yao and Dennis Klug, *Phys. Rev. B* 2015, **91**, 014102