

First-principles study of solid iron-hydrogen alloys under high pressure

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Hydrogen and iron are two of major constituents of the Earth and planetary interiors. The crystal structure of solid FeH_x is one of the most fundamental information in order to understand properties of planetary cores. Recently, hydrogen-rich phases, FeH₂ and FeH₃, were experimentally synthesized [1]. The crystal structure of FeH₃ was clarified by comparing experimental compression curve with calculated one. On the other hand, the structure of FeH₂ remains unclear. It is mainly because the hydrogen positions are quite difficult to be determined by x-ray diffraction measurements. Ref. 1 proposed the crystal structure of FeH₂, but it is less consistent with its experimental compression curve. Here we report the results of first-principles calculations on FeH₂. We find the new hydrogen positions which lead to more stable structure than proposed by Ref. 1 and reproduces experimental compression curve very well. Our new structure will be essential for constraining the amount of hydrogen in iron alloys.

[1] C. M. Pépin, A. Dewaele, G. Geneste, P. Loubeyre, and M. Mezouar, Phys. Rev. Lett. 113, 265504 (2014).

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