Solid iron-hydrogen alloys under high pressure by first principles

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Since hydrogen and iron are two of major constituents of the Earth and planetary interiors, the crystal structures of hydrogen-bearing iron solid are one of the most fundamental information in order to understand properties of planetary cores. Recently, hydrogen-rich phases, FeH_2 and FeH_3, were experimentally synthesized [1]. The crystal structure of FeH_3 was clarified by comparing experimental compression curve with calculated one. On the other hand, the structure of FeH_2 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 FeH_2 with the iron sublattice symmetry of I4/mmm, but it is less consistent with its experimental compression curve. Here we report the results of first-principles calculations on FeH_2. We find the new hydrogen positions which lead to more stable structure than proposed by Ref. 1 and reproduces experimental compression curve very well. Combined with the crystal structures of FeHx for x<1 which have been well known, we will have volume per hydrogen in iron-hydrogen alloys. It will be an essential information to determine the amount of hydrogen.

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