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 FeHx is 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, 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. Our new structure will be essential for constraining the amount of hydrogen in iron alloys.
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