First-principles prediction of the structural, elastic and mechanical properties of of hydrides Ba2RuH6

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Abstract : We report a systematic study of the structural, elastic and mechanical properties of the ternary ruthenium-based hydrides Ba2RuH6 within first-principles approach. The elastic behavior of a cubic monocrystalline is characterized completely by ¶three elastic constant independent C11, C12 and C44.We note here the absence of any experimental or theoretical data on the single-crystal and polycrystalline elastic moduli and their related properties elastic constants for the studied materials to be compared with our findings.

Keywords : Ruthenium-based hydrides; First-principles calculations; Elastic constants; Mechanical properties.