

# First-principles prediction of the structural, elastic and mechanical properties of of hydrides $\text{Ba}_2\text{RuH}_6$

**O. Boudrifa, A. Bouhemadou**

**Abstract :** We report a systematic study of the structural, elastic and mechanical properties of the ternary ruthenium-based hydrides  $\text{Ba}_2\text{RuH}_6$  within first-principles approach. The elastic behavior of a cubic monocrystalline is characterized completely by three elastic constant independent  $C_{11}$ ,  $C_{12}$  and  $C_{44}$ . 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.