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Structural, Elastic, Vibrational and Thermal Properties of Perovskites AHfO3 (a=Ba,Sr,Eu)

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Abstract : The structural, elastic, vibrational and thermal properties of AHfO3 compounds with the cubic perovskites structure have been investigated, by employing a first principles method, using the plane wave pseudo potential calculations (PP-PW), based on the density functional theory (DFT), within the local density approximation (LDA). The optimized lattice parameters, independent elastic constants (C11, C12 and C44), bulk modulus (B), compressibility (b), shear modulus (G), Young's modulus (Y), Poisson's ratio (n), Lame´'s coefficients (m, l), as well as band structure, density of states and electron density distributions are obtained and analyzed in comparison with the available theoretical and experimental data. For the first time the numerical estimates of elastic parameters of the polycrystalline AHfO3 ceramics (in framework of the VoigteReusseHill approximation) are performed. The quasi-harmonic Debye model, by means of total energy versus volume calculations obtained with the FP-LAPW method, is applied to study the thermal and vibrational effects. Predicted temperature and pressure effects on the structural parameters, thermal expansions, heat capacities, and Debye temperatures are determined from the non-equilibrium Gibbs functions.

Keywords : Hafnium, elastic propreties, first principles calculation, perovskite
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