European Journal of Chemistry 16 (3) (2025) 292-301

Supplementary Materials

Comprehensive DFT analysis of $BeHfO_3$ perovskite: Exploring the structure, mechanical, thermodynamic, and optic properties

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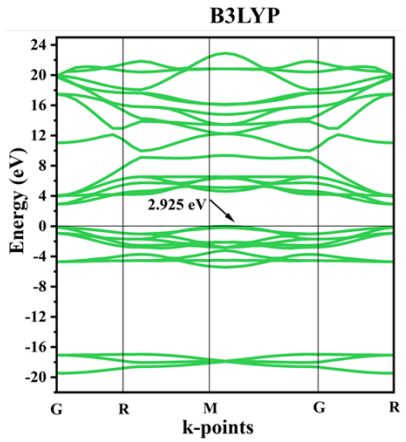

Figure S1. Band structure of $BeHfO_3$ using B3LYP method.

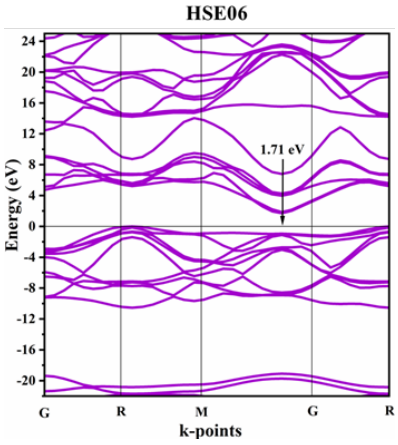

Figure S2. Band structure of $BeHfO_3$ using HSE06 method.

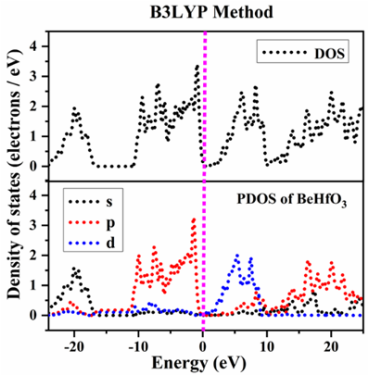

Figure S3. DOS and PDOS of $BeHfO_3$ using B3LYP method.

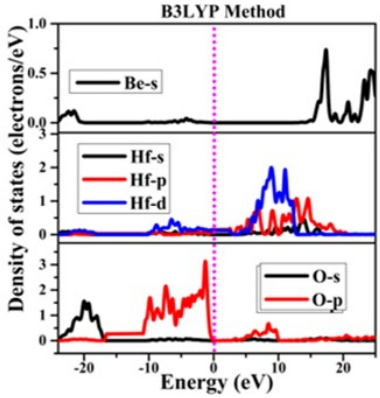

Figure S4. Different partial states of $BeHfO_3$ using B3LYP method.

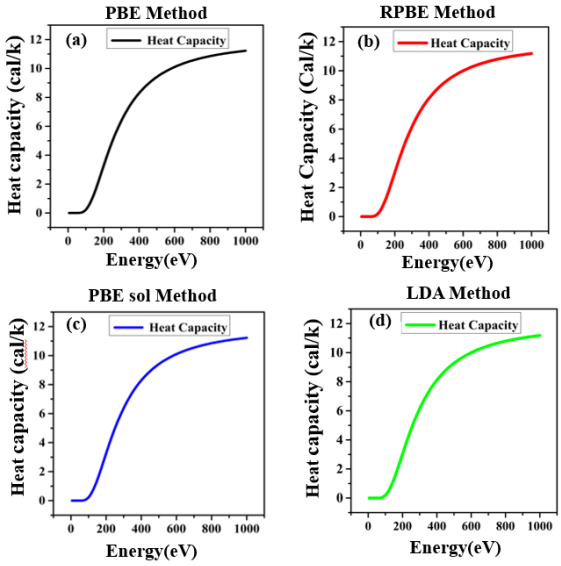

Figure S5. Heat capacity of $BeHfO_3$ in (a) PBE (b) RPBE (c) PBE sol and (d) LDA methods.

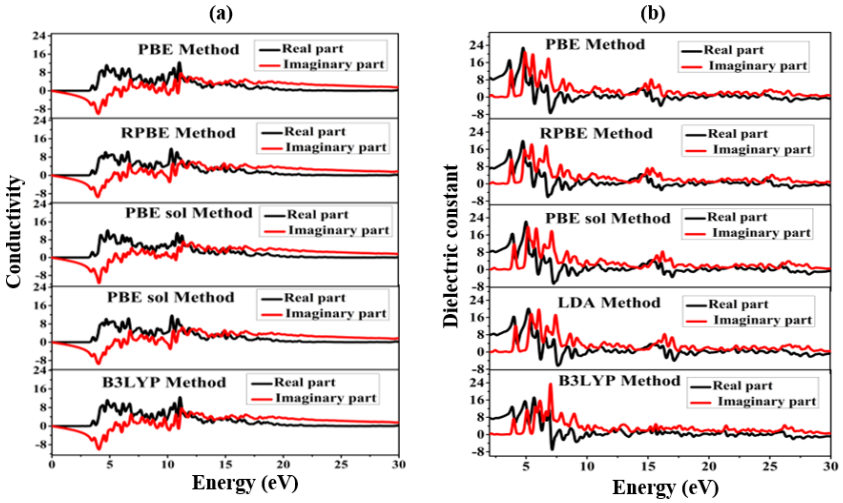

Figure S6. (a) Optical conductivity and (b) Dielectric function of $BeHfO_3$ in GGA using the PBE, RPBE, PBE sol, LDA and B3LYP Methods.

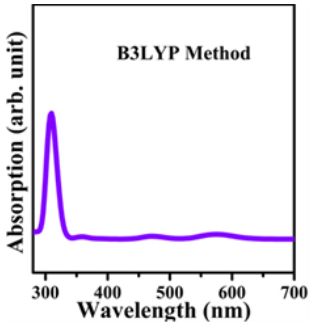

Figure S7. Optical Absorption of $BeHfO_3$ using B3LYP method.