

Electronic Supplementary Information (ESI)

Predicting Band Gaps of ABN_3 Perovskites: An Account from Machine Learning and First-Principle DFT Studies

Swarup Ghosh and Joydeep Chowdhury*

Affiliation

Department of Physics, Jadavpur University, 188, Raja S.C. Mallick Road, Kolkata
700032, India

***Corresponding Author:** joydeep72_c@rediffmail.com /

joydeep.chowdhury@jadavpuruniversity.in

Table S1. List of 117 features in predicting band gaps of ABN₃ perovskite compounds.

Mendelev number min/ max/ range/ mean/ avg_dev/ mode	Atomic weight min/ max/ range/ mean/ avg_dev/ mode	Melting temperature min/ max/ range/ mean/ avg_dev/ mode
Covalent radius min/ max/ range/ mean/ avg_dev/ mode	Electronegativity min/ max/ range/ mean/ avg_dev/ mode	s valence electrons min/ max/ range/ mean/ avg_dev/ mode
p valence electrons min/ max/ range/ mean/ avg_dev/ mode	d valence electrons min/ max/ range/ mean/ avg_dev/ mode	f valence electrons min/ max/ range/ mean/ avg_dev/ mode
Total valence electrons min/ max/ range/ mean/ avg_dev/ mode	Unfilled s states min/ max/ range/ mean/ avg_dev/ mode	Unfilled p states min/ max/ range/ mean/ avg_dev/ mode
Unfilled d states min/ max/ range/ mean/ avg_dev/ mode	Unfilled f states min/ max/ range/ mean/ avg_dev/ mode	Total unfilled states min/ max/ range/ mean/ avg_dev/ mode
Specific volume per atom of ground state min/ max/ range/ mean/ avg_dev/ mode	Band gap energy of ground state min/ max/ range/ mean/ avg_dev/ mode	Magnetic moment of ground state min/ max/ range/ mean/ avg_dev/ mode
Space group number min/ max/ range/ mean/ avg_dev/ mode	Ionic character max/ mean	Formation energy

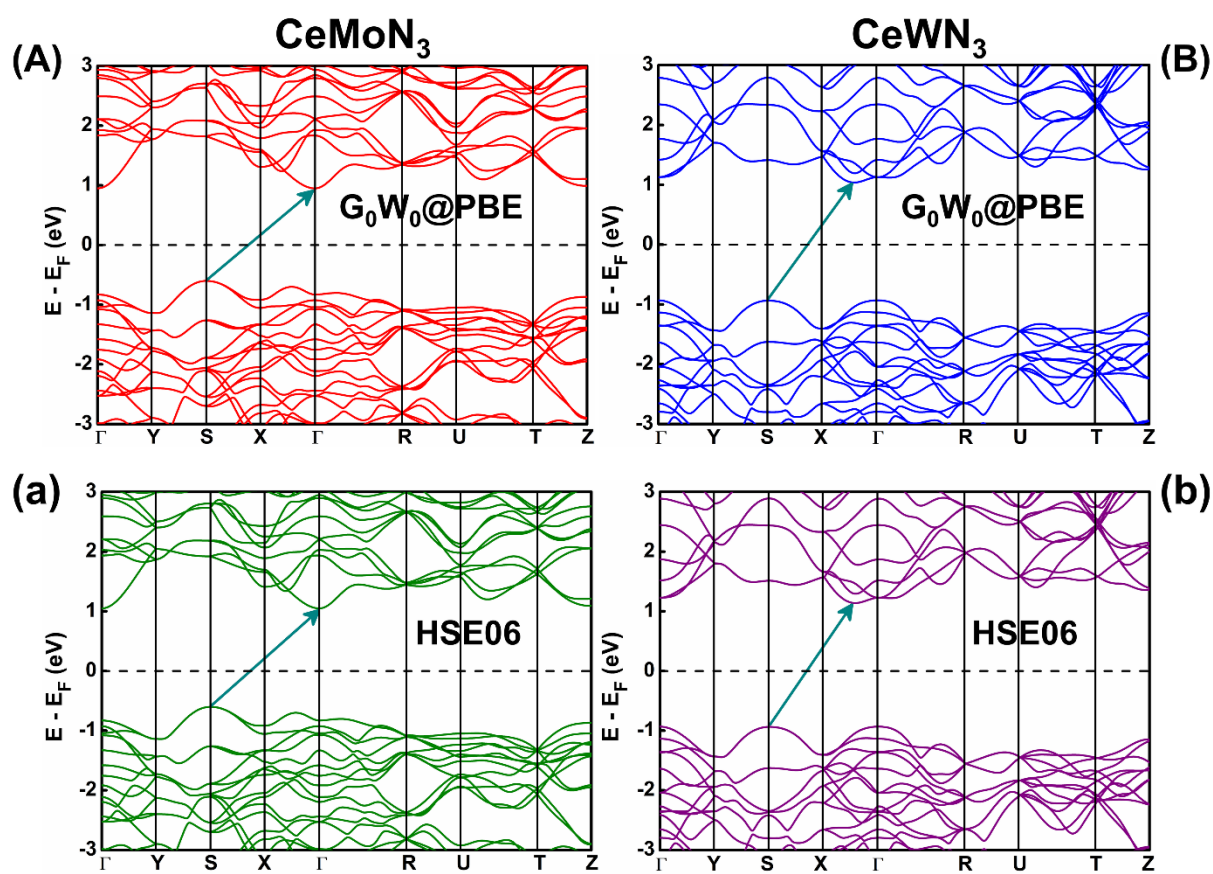


Fig. S1. E-k diagrams of $CeMoN_3$ (left panel) and $CeWN_3$ (right panel) compounds along $\Gamma \rightarrow Y \rightarrow S \rightarrow X \rightarrow \Gamma \rightarrow R \rightarrow U \rightarrow T \rightarrow Z$ high-symmetry direction as obtained from $G_0W_0@PBE$ and HSE06 level of theories [Horizontal dashed line and inclined arrow represent Fermi energy level and band gap, respectively].