

Supporting Information

Insulator-to-Metal Transition, Magnetic Anisotropy, and Improved T_C in a Ferrimagnetic $\text{La}_2\text{CoIrO}_6$: Strain Influence

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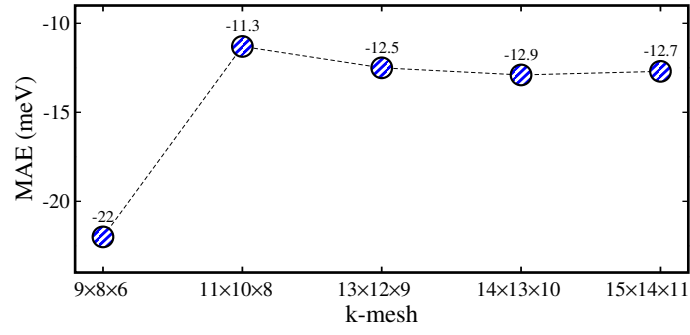


FIG. 1S: (Color online) Computed magnetocrystalline anisotropy energy (MAE) as a function of various k-meshes in the $\text{La}_2\text{CoIrO}_6$ double perovskite oxide.

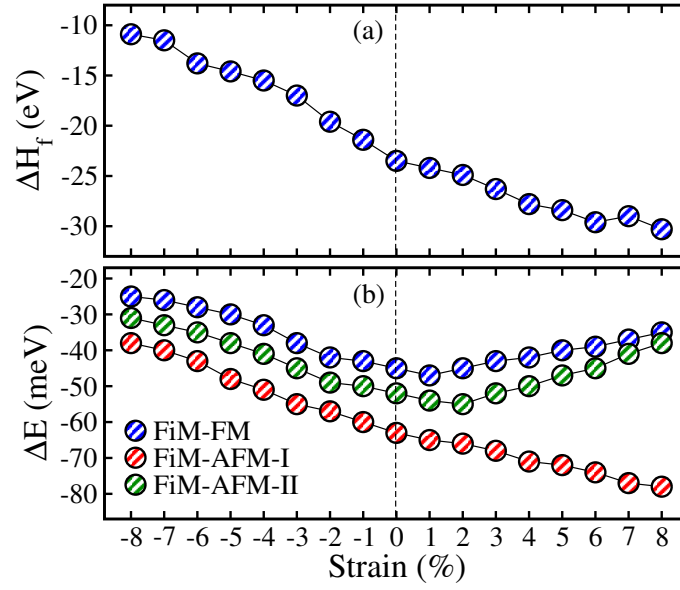


FIG. 2S: (Color online) Computed (a) enthalpies of formation (ΔH_f) and (b) total energy differences (ΔE) of ferrimagnetic (FiM) with ferromagnetic (FM)/anti-ferromagnetic-I (AFM-I)/(AFM-II) spin ordering with respect to $\pm 8\%$ biaxial ($[110]$) strain along the ab -plane in the $\text{La}_2\text{CoIrO}_6$ double perovskite oxide.

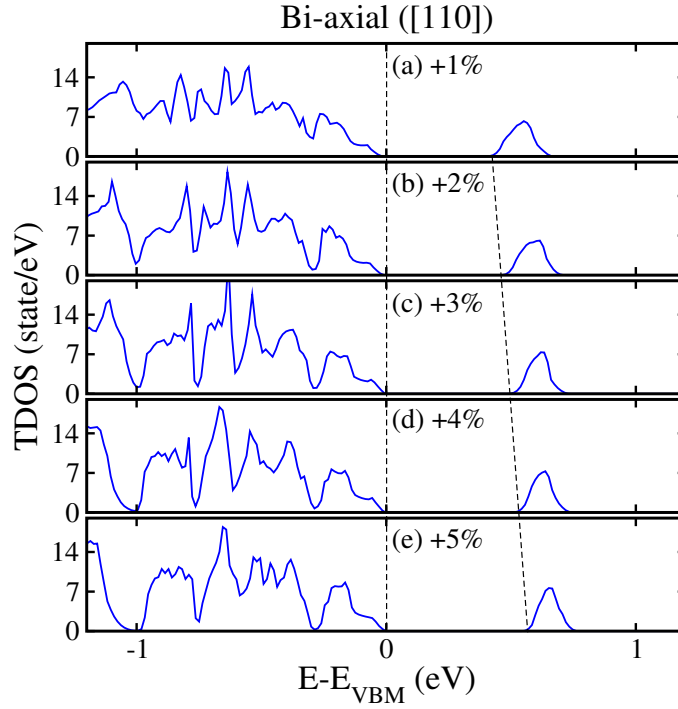


FIG. 3S: (Color online) Computed GGA+ U +SOC spin non-degenerate total density of states for (a) +1%, (b) +2%, (c) +3%, (d) +4%, and (e) +5% biaxial ([110]) tensile strains along the ab -plane in the stable ferrimagnetic spin-ordering of $\text{La}_2\text{CoIrO}_6$ double perovskite oxide.

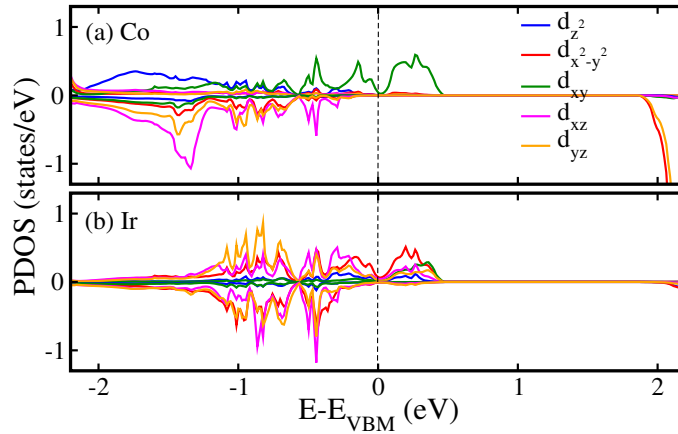


FIG. 4S: (Color online) Computed GGA+ U +SOC spin non-degenerate 3 d -orbital resolved partial density of states (PDOS) for a critical -6% biaxial ([110]) compressive strain along the ab -plane of (a) Co and (b) Ir ions in the stable ferrimagnetic spin-ordering of $\text{La}_2\text{CoIrO}_6$ double perovskite oxide.