Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supporting Information

Stable Antiferromagnetism and Semiconducting-to-Metal Transition in ALaCuOsO$_6$ (A = Ba and Sr): Strain Modulations

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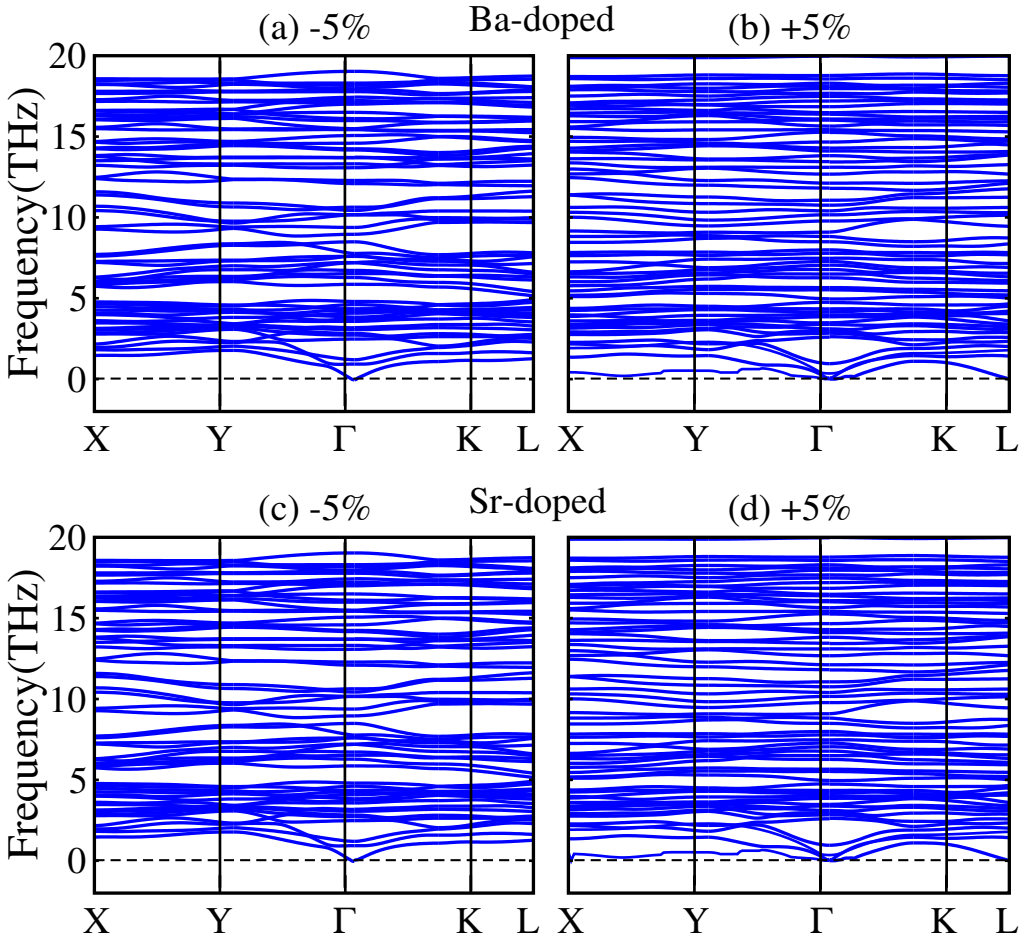

FIG. 1S: (Color line) Calculated phonon dispersion band structures for (a/c) −5% and (b/d) +5% in Ba- (first row)/Sr- (second row) doped La_2CuOsO_6 double perovskite oxides.

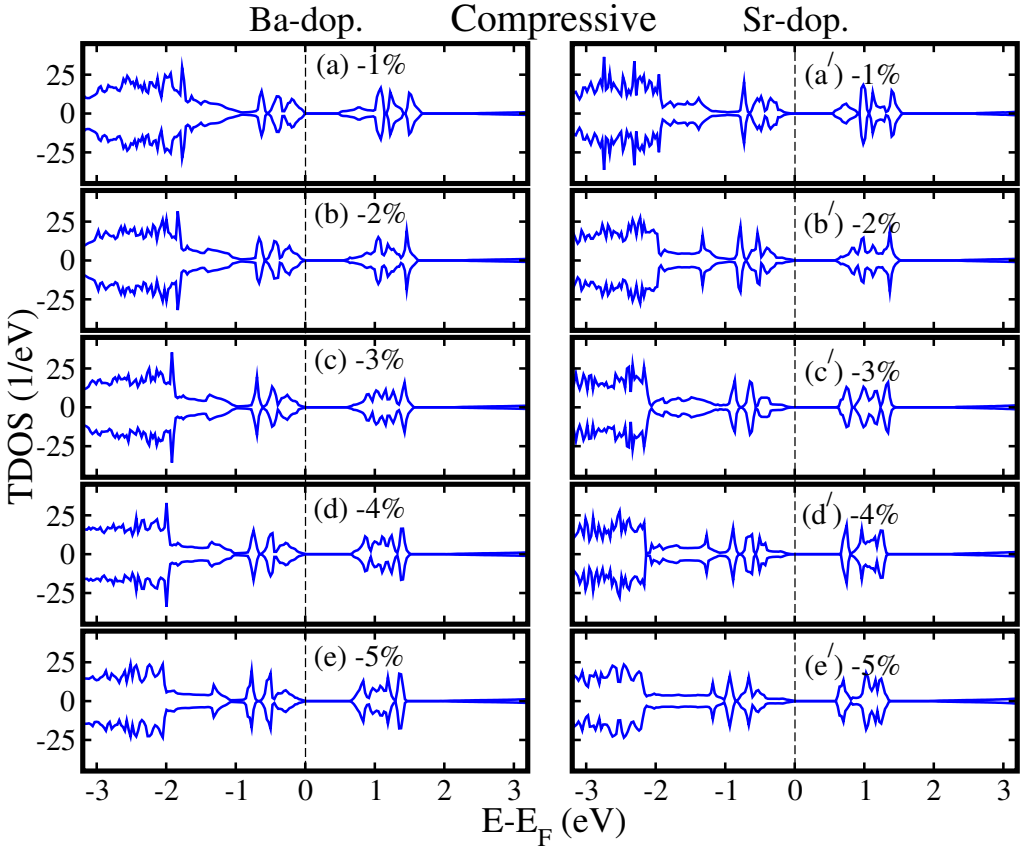

FIG. 2S: (Color line) GGA+U+SOC calculated spin-polarized total density of states for (a and a′) −1%, (b and b′) −2%, (c and c′) −3%, (d and d′) −4%, and (e and e′) −5% biaxial compressive strains along the [110]-direction in the most stable antiferromagnetic spin ordering of Ba- (left column) and Sr- (right column) doped La_2CuOsO_6 double perovskite oxides.

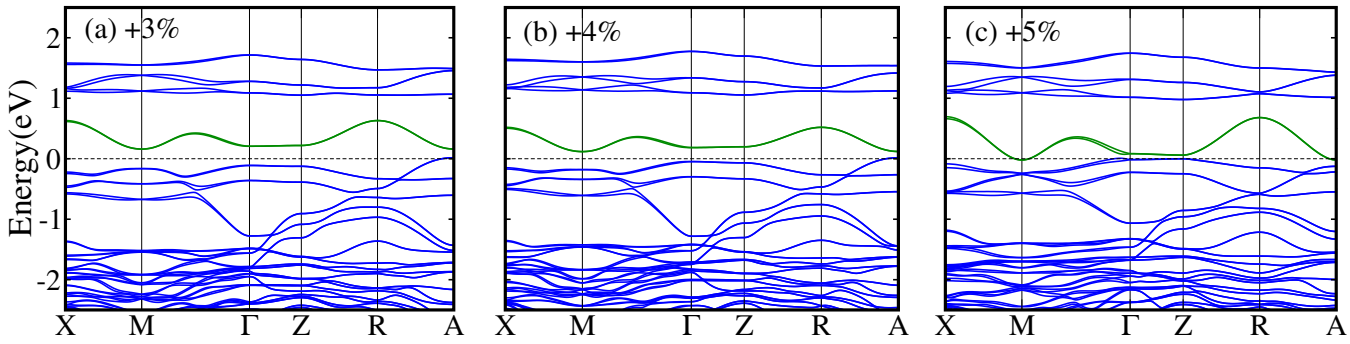

FIG. 3S: (Color online) GGA+U+SOC calculated spin-polarized band structures for (a) +3%, (a) +4%, and (c) +5% biaxial tensile strains along the [110]-direction in the most stable antiferromagnetic spin ordering of Sr-doped La_2CuOsO_6 double perovskite oxide. For clarity, a few bands are highlighted with green colors which are near/at the Fermi level in each case.

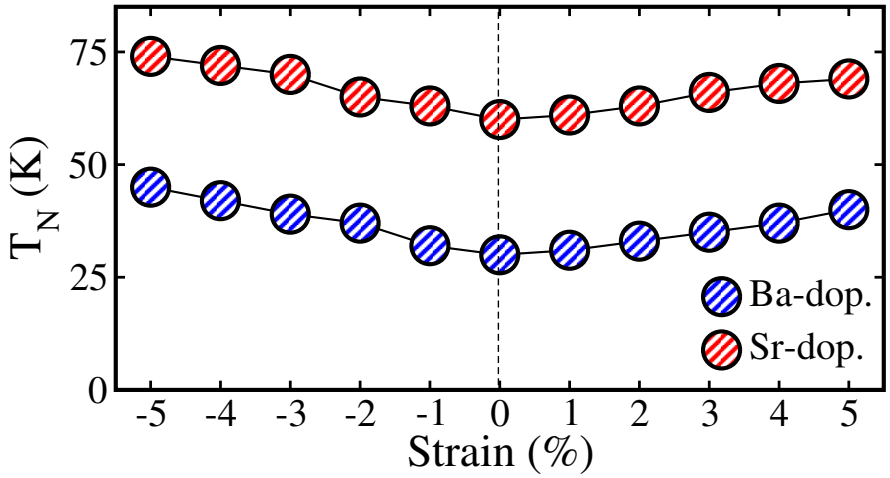

FIG. 4S: (Color line) Calculated Neel temperature (T_N) as a function of biaxial strains having ranged from -5% to $+5\%$ along the [110]-direction in the most stable antiferromagnetic spin ordering of Ba- and Sr-doped La_2CuOsO_6 double perovskite oxides.