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Supporting Information

Interplay between Spin-Orbital Coupling and Electron Correlation: Induction of Phase Transitions and Giant Magnetic Anisotropy in Strained $LaSr_{1-x}Ca_xNiReO_6$

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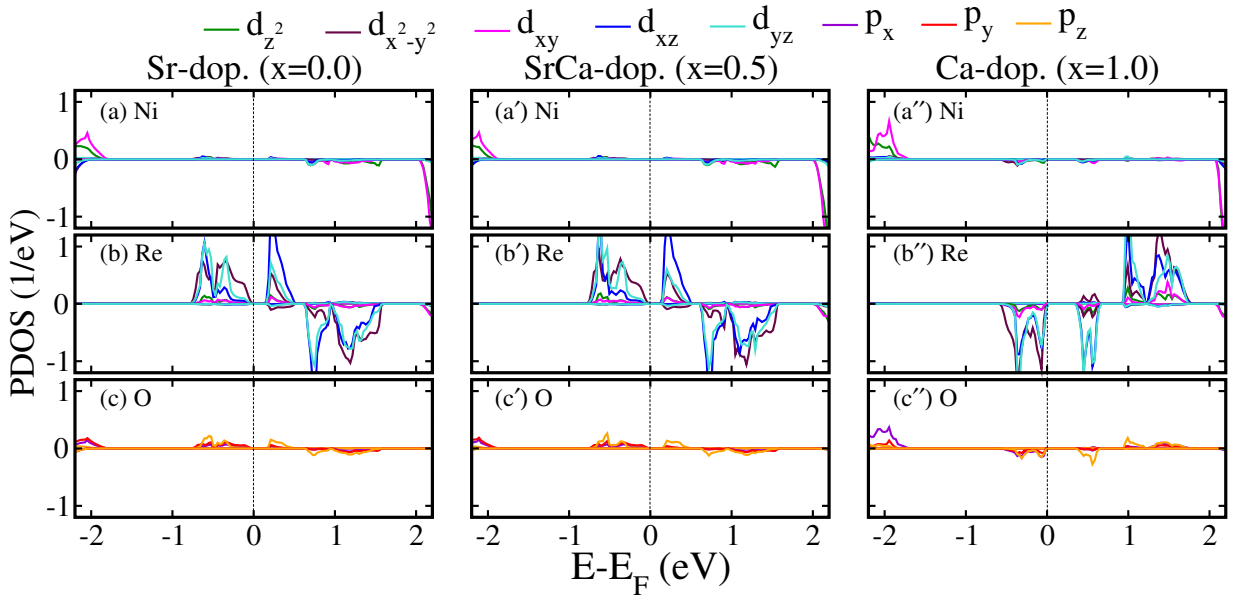

FIG. 1S: Calculated spin-polarized partial density of states (PDOS) within a GGA+U+SOC method for (a/a′/a″) Ni $3d$ (first row), (b/b′/b″) Re $5d$ (second row), and (c/c′/c″) O $2p$ (third row) orbitals of Sr-dop. ($x = 0.0$) in the left column/SrCa-dop. ($x = 0.5$) in the middle column/Ca-dop. ($x = 1.0$) in the right column in unstrained $LaSr_{1-x}Ca_xNiReO_6$ ($x = 0.0/0.5/1.0$)) double perovskite oxide, respectively.

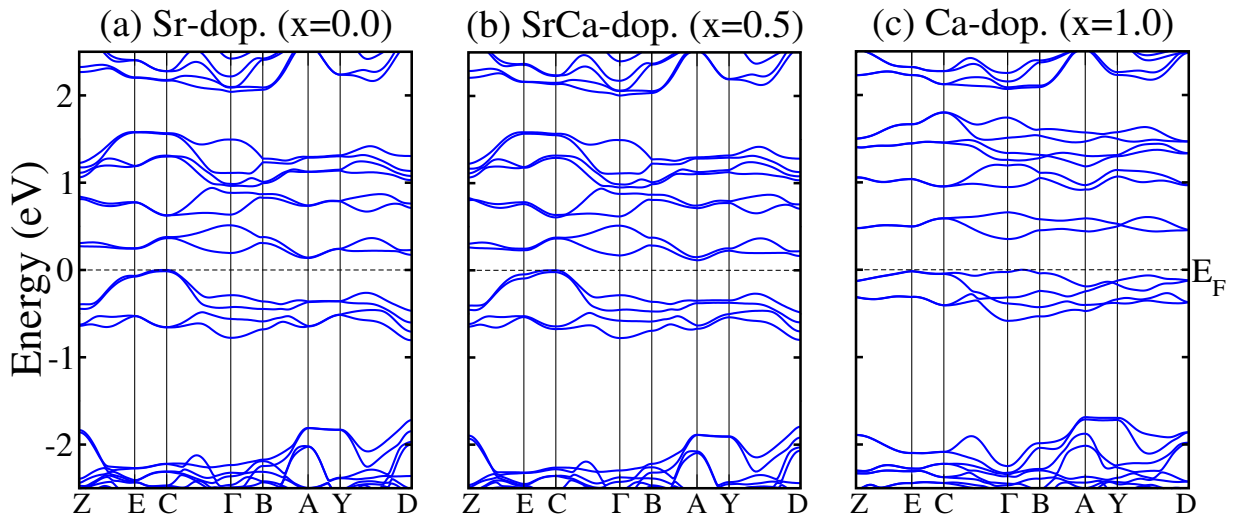

FIG. 2S: Calculated band structures of the $LaSr_{1-x}Ca_xNiReO_6$ double peroveskite oxide for (a) Sr-dop. ($x = 0.0$), (b) SrCa-dop. ($x = 0.5$), and (c) Ca-dop. ($x = 1.0$) within the GGA+U+SOC method in the respective stable magnetic ground states in each case. For clarity, the horizontal dotted line represents the Fermi level.

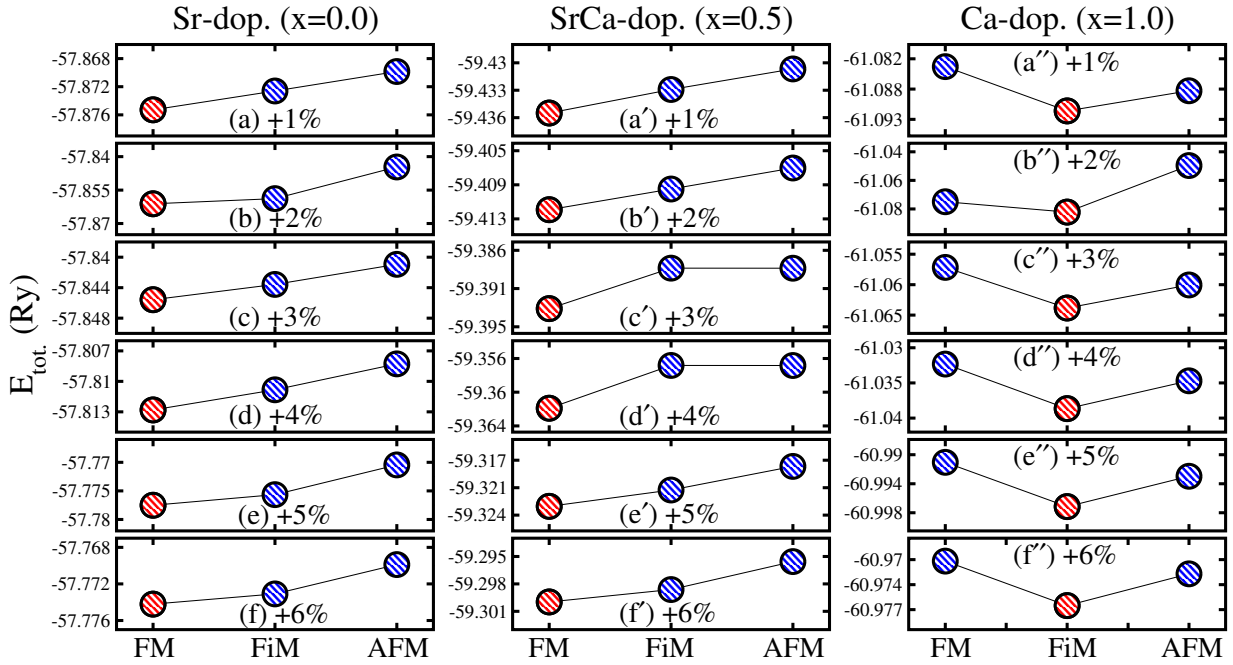

FIG. 3S: (Color online) Calculated total magnetic energies ($E_{tot.}$) of the $LaSr_{1-x}Ca_xNiReO_6$ double peroveskite oxide for (a/b/c/d/e/f) Sr-dop. ($x = 0.0$) in the left column, (a′/b′/c′/d′/e′/f′) SrCa-dop. ($x = 0.5$) in the middle column, and (a″/b″/c″/d″/e″/f″) Ca-dop. ($x = 1.0$) in the right column for biaxial tensile +1%/+2%/+3%/+4%/+5%/+6% strains along the [110]-direction as a function of ferromagnetic (FM)/ferrimagnetic (FiM)/antiferromagnetic (AFM) spin ordering within GGA+U+SOC method. For clarity, the magnetic ground states in each case are visualized by the red circles.

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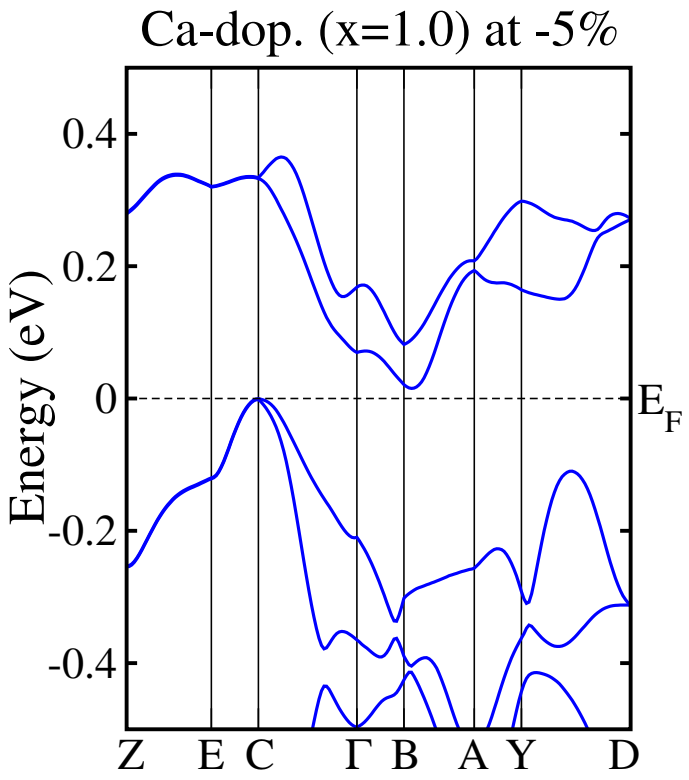

FIG. 4S: (Color online) Calculated band structures of the $LaSr_{1-x}Ca_xNiReO_6$ double perovskite oxide for Ca-dop. ($x = 1.0$) within the GGA+U+SOC method in the respective stable magnetic ground state at a critical strain of -5% compressive strain.

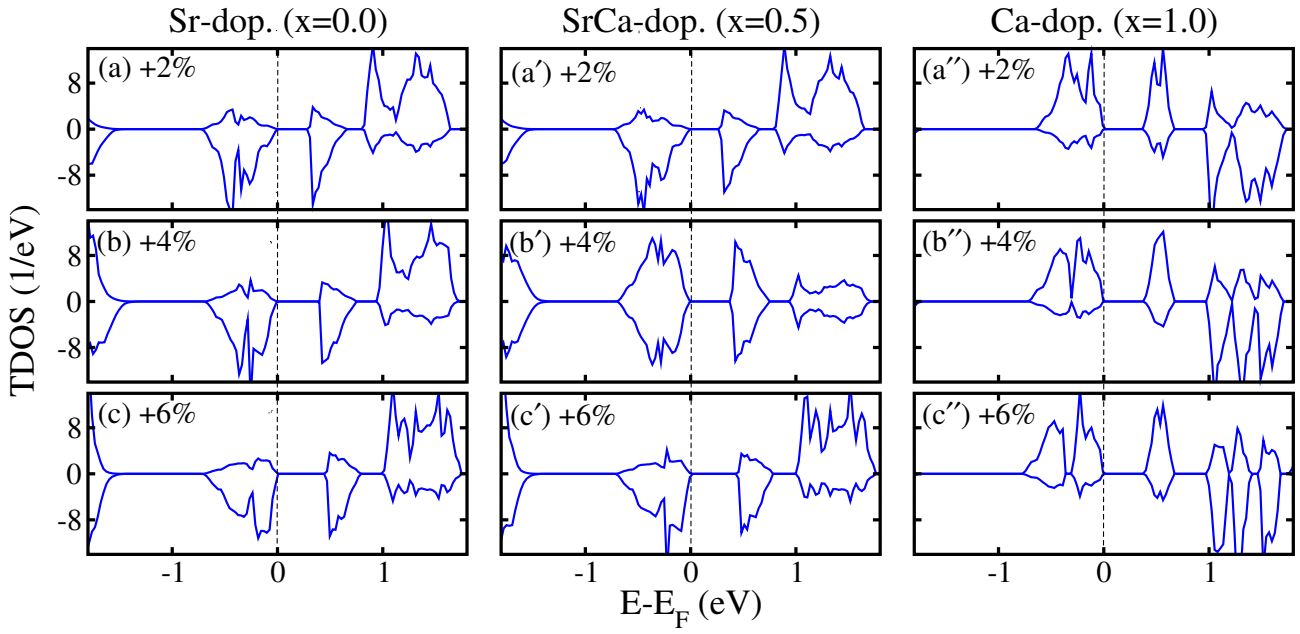

FIG. 5S: (Color online) Calculated spin-polarized total density of states (TDOS) of the $LaSr_{1-x}Ca_xNiReO_6$ double peroveskite oxide for (a/b/c) Sr-dop. ($x = 0.0$) in the left column, (a′/b′/c′) SrCa-dop. ($x = 0.5$) in the middle column, and (a″/b″/c″) Ca-dop. ($x = 1.0$) in the right column as a function of biaxial tensile +2%/+4%/+6% strains along the [110]-direction within GGA+U+SOC method.

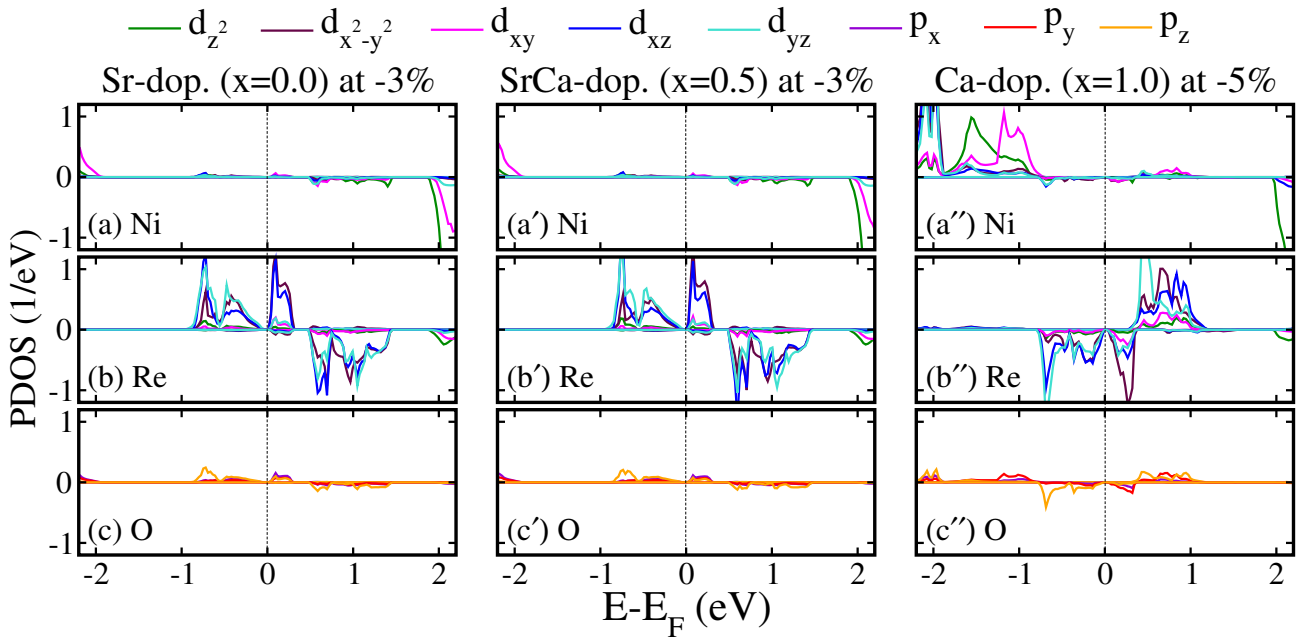

FIG. 6S: (Color online) Calculated spin-polarized partial density of states (PDOS) within a GGA+U+SOC method for (a/a′/a″) Ni $3d$ (first row), (b/b′/b″) Re $5d$ (second row), and (c/c′/c″) O $2p$ (third row) orbitals Sr-dop. ($x = 0.0$) in the left column/SrCa-dop. ($x = 0.5$) in the middle column/Ca-dop. ($x = 1.0$) in the right column in unstrained $LaSr_{1-x}Ca_xNiReO_6$ double perovskite oxides, respectively.

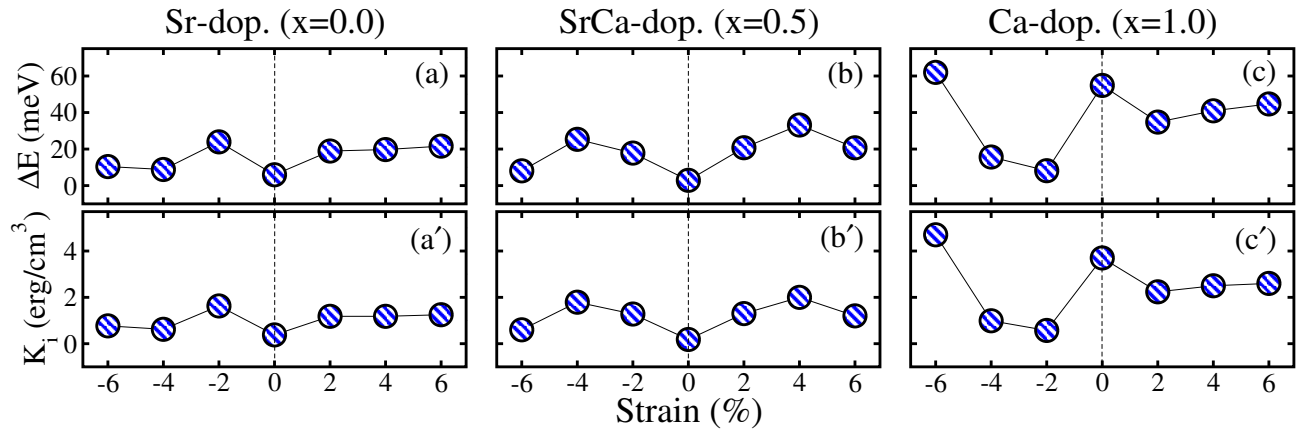

FIG. 7S: (Color online) Calculated ΔE (the difference between the two consecutive lowest energy levels along with the crystallographic axis in which the spin magnetization is applied) in the first row and K_i (the magnetocrystalline anisotropy energy constant) in the second row as a function of biaxial strain along the [110]-direction of the $LaSr_{1-x}Ca_xNiReO_6$ double perovskite oxide for (a and a′) Sr-dop. ($x = 0.0$) in the first column, (b and b′) SrCa-dop. ($x = 0.5$) in the second column, and (c and c′) Ca-dop. ($x = 1.0$) in the third column within the GGA+U+SOC method in the respective stable magnetic ground states.

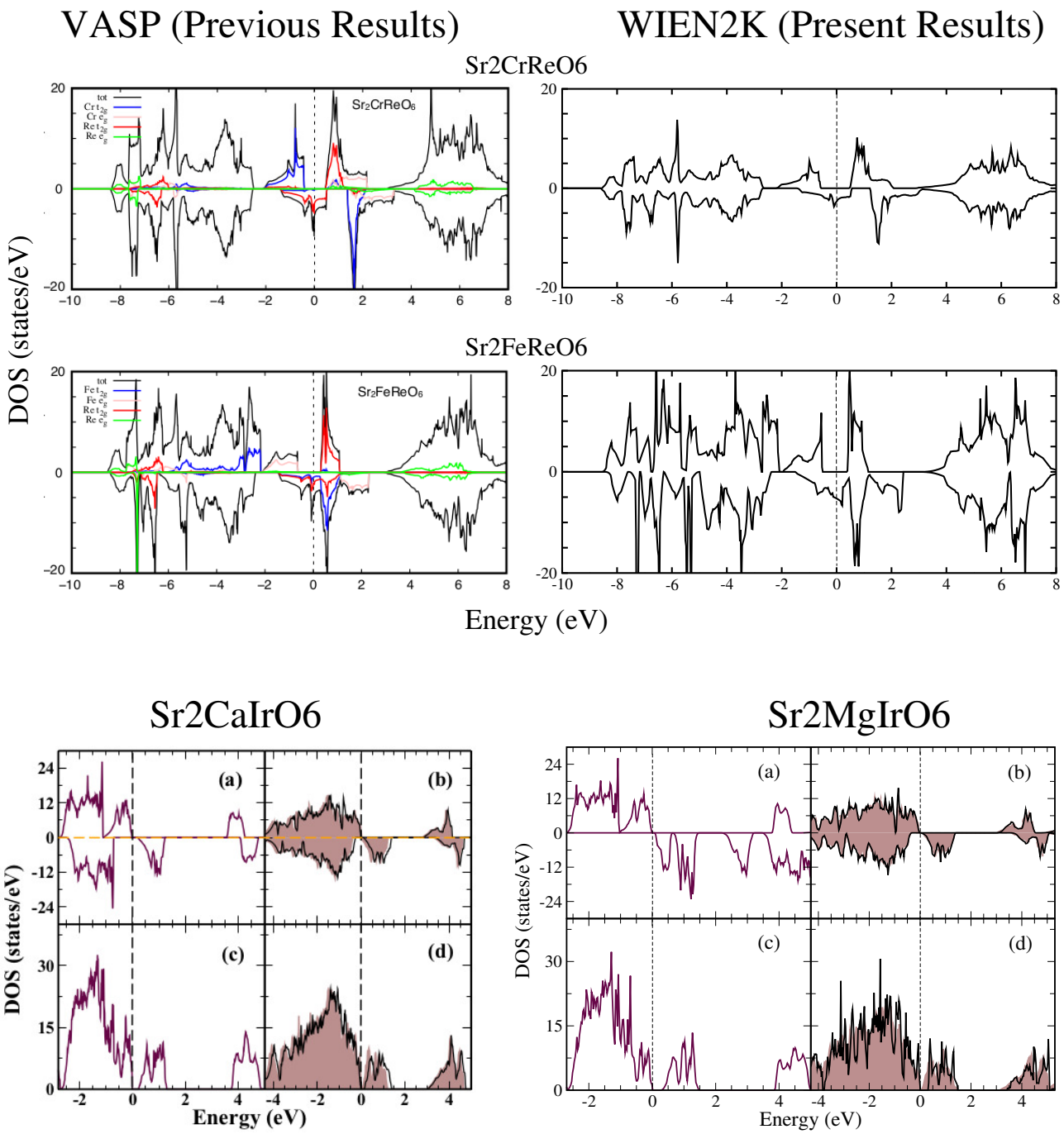

FIG. 8S: (Color online) A comparison of the calculated density of states (DOS) using VASP (previous results) in the left column and WIEN2K (present results) in the right column for different four double perovksite oxides such as Sr_2CrReO_6, Sr_2CrFeO_6, Sr_2CaIrO_6, and Sr_2MgIrO_6.