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

Supporting Information

Strain-Driven Half-Metallicity in a Ferri-Magnetic Mott-Insulator Lu_2NiIrO_6: A First-Principles Perspective

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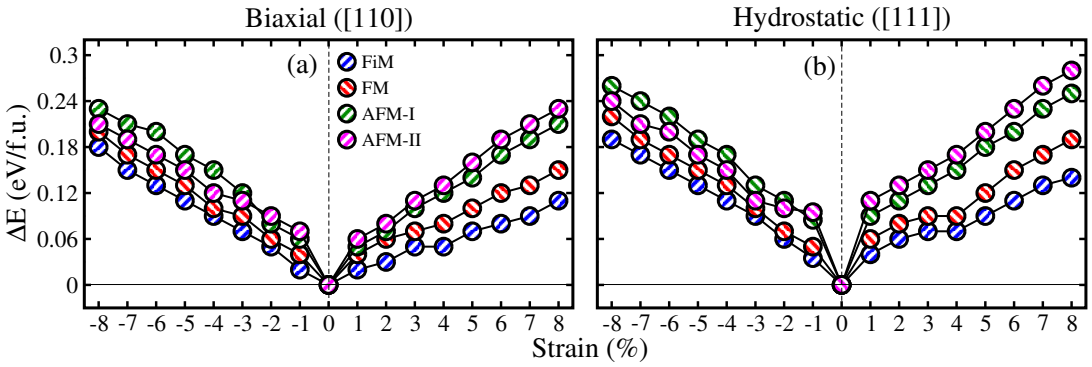

FIG. 1S: Comparison of strain dependence structural stability (*i. e.,* energy versus strain) of the four magnetic spin ordering: (1) ferromagnetic (FM), (2) ferrimagnetic (FiM), (3) antiferromagnetic-I (AFM-I), and (4) antiferromagnetic-II (AFM-II) in Lu_2NiIrO_6 double perovskite oxide with in GGA+U+SOC method for (a) biaxial ([110]) (b) hydrostatic ([111]) strains.

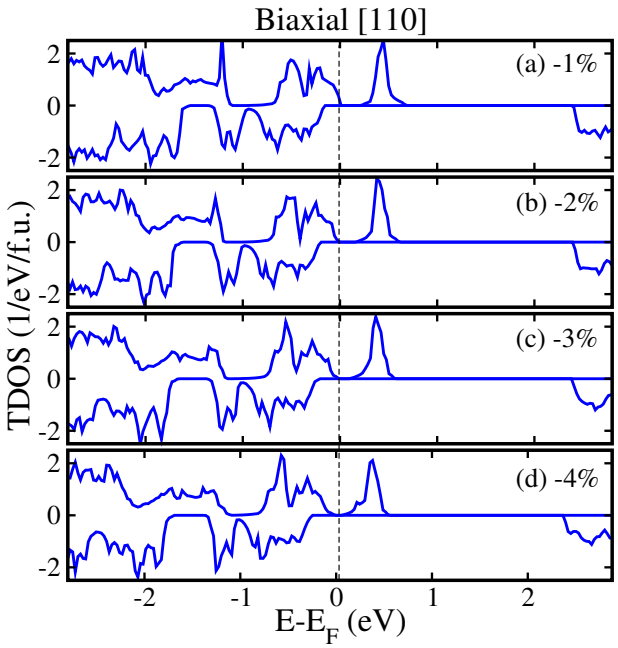

FIG. 2S: Calculated spin-polarized total density of states (TDOS) of Lu_2NiIrO_6 DPO for (a) -1%, (b) -2%, (c) -3%, and (d) -4% biaxial compressive strains along [110]-direction.

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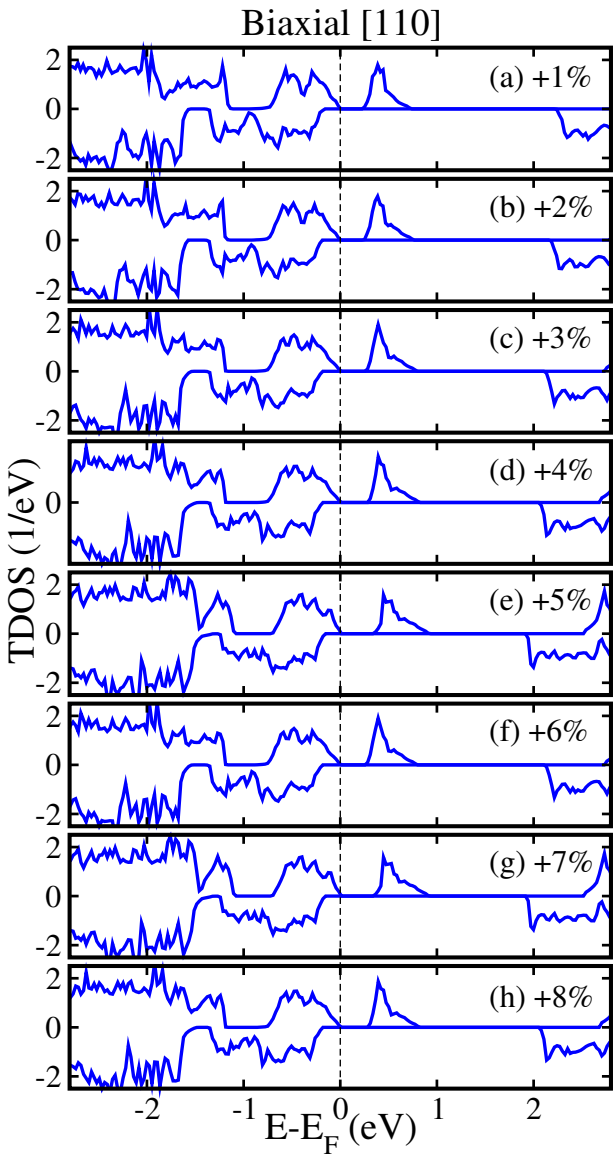

FIG. 3S: Calculated spin-polarized total density of states (TDOS) of Lu_2NiIrO_6 DPO for (a) +1%, (b) +2%, (c) +3%, (d) +4%, (e) +5%, (f) +6%, (g) +7%, and (h) +8% biaxial tensile strains along [110]-direction.

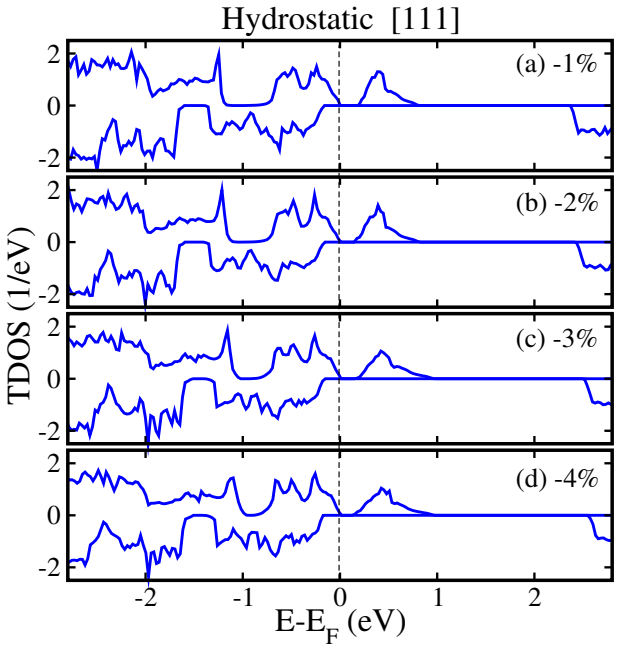

FIG. 4S: Calculated spin-polarized total density of states (TDOS) of Lu_2NiIrO_6 DPO for (a) -1%, (b) -2%, (c) -3%, and (d) -4% hydrostatic compressive strains along [111]-direction.

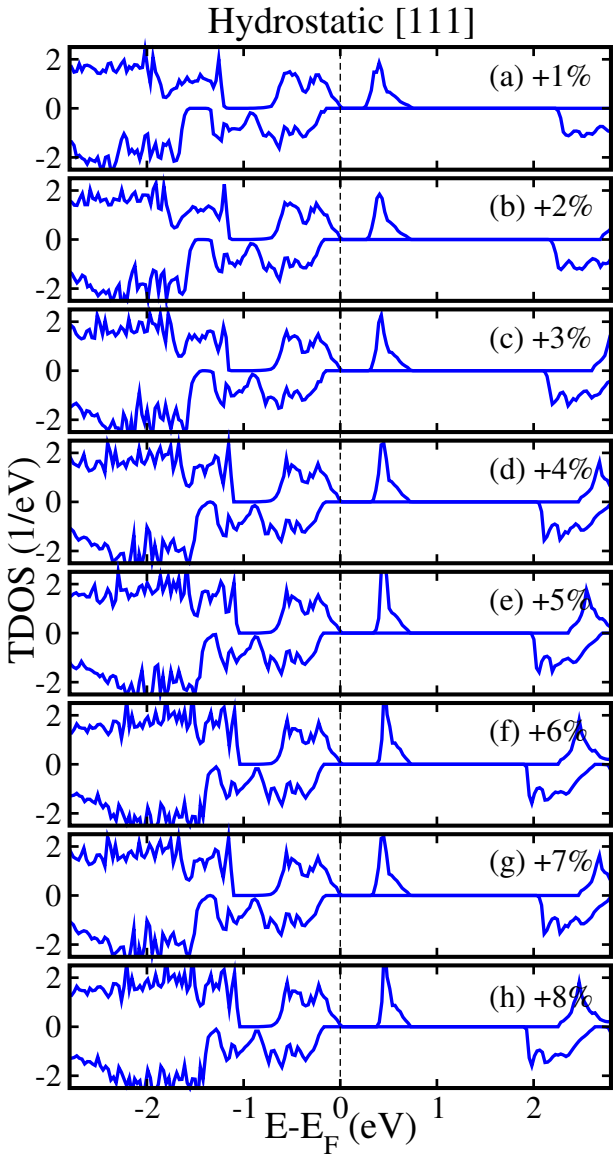

FIG. 5S: Calculated spin-polarized total density of states (TDOS) of Lu_2NiIrO_6 DPO for (a) +1%, (b) +2%, (c) +3%, (d) +4%, (e) +5%, (f) +6%, (g) +7%, and (h) +8% hydrostatic tensile strains along [111]-direction.

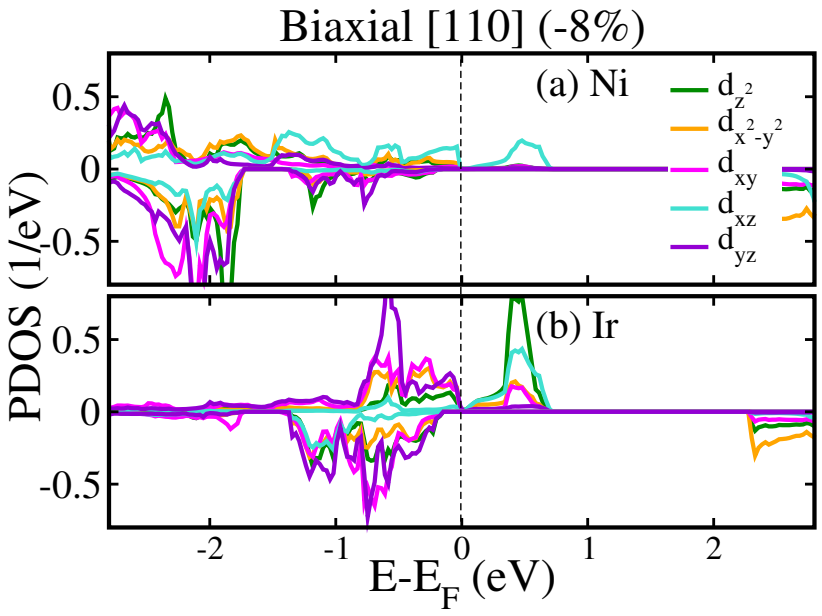

FIG. 6S: Calculated spin-polarized orbital resolved partial density of states (PDOS) for (a) Ni $3d$ and (b) Ir $5d$ orbitals of Lu_2NiIrO_6 DPO for -8% biaxial compressive strain.

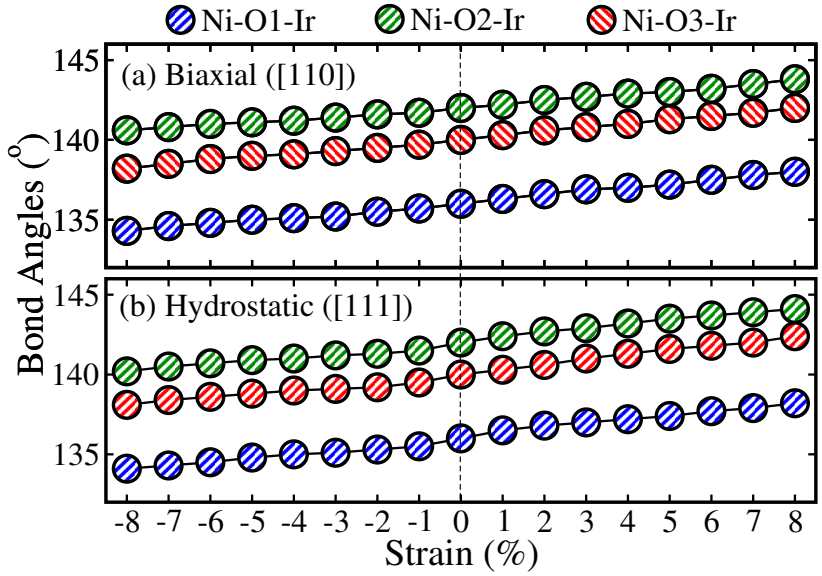

FIG. 7S: Calculated Ni-O1-Ir, Ni-O2-Ir, and Ni-O3-Ir bond angles of Lu_2NiIrO_6 DPO as a function of (a) biaxial ([110]) and (b) hydrostatic ([111]) strains.

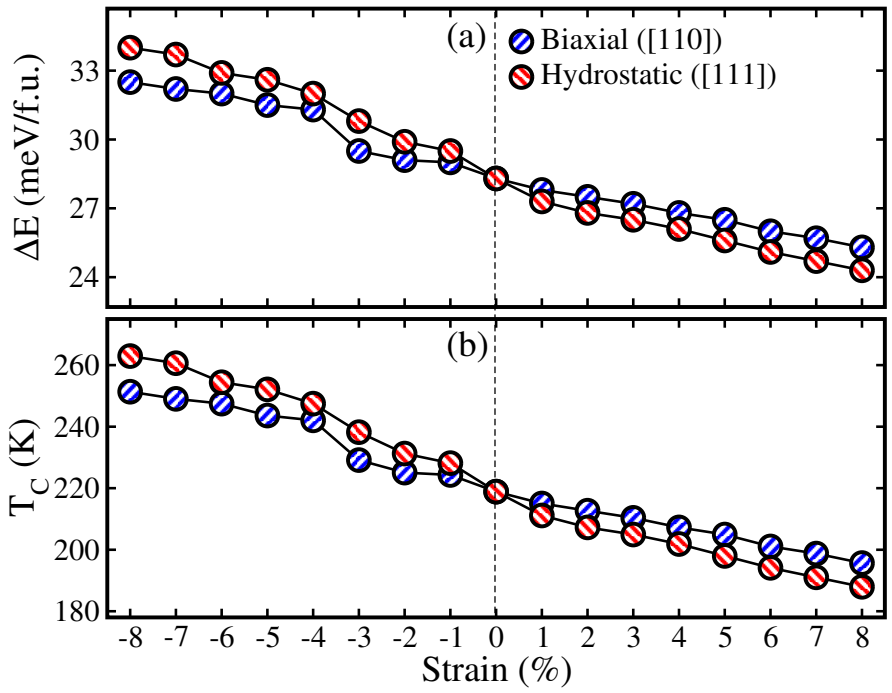

FIG. 8S: Calculated (a) $\Delta E = E_{FiM} - E_{FM}$ (energy difference between ferrimagnetic (FiM) and ferromagnetic (FM) spin ordering) and (b) magnetic transition temperature (T_C) as a function of biaxial ([110] and hydrostatic ([111]) strains.