Supporting Information

Structural Stability and Evolution of Half-Metallicity in Ba_2CaMoO_6: Interplay of Hole- and Electron-Doping

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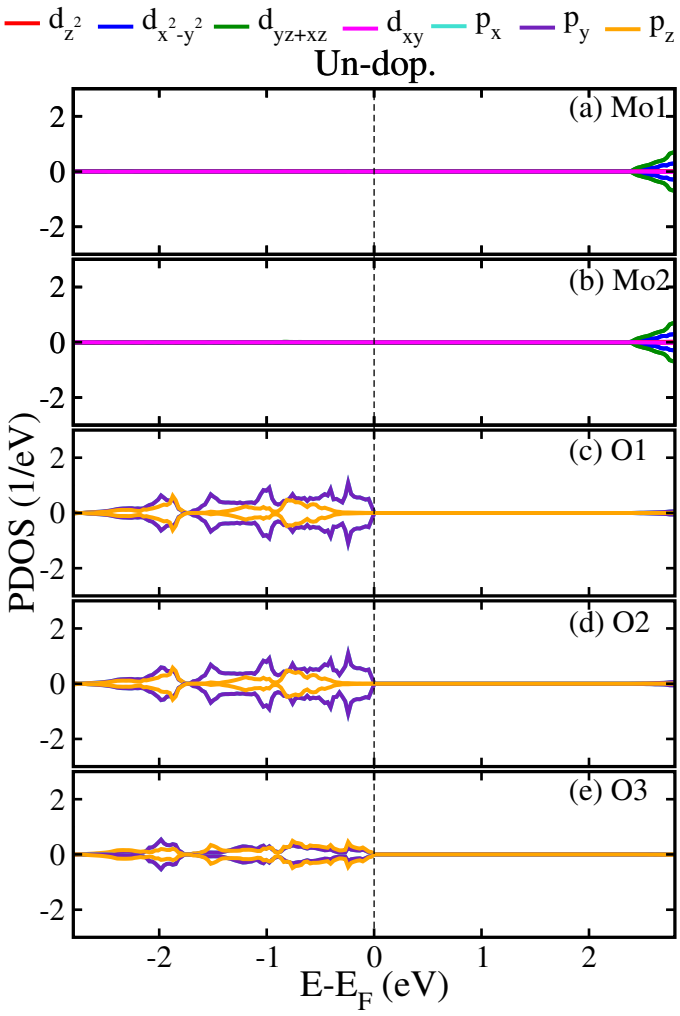

FIG. 1S: Calculated spin-polarized (a) Mo1, (b) Mo2 4*d*, (c) O1, (d) O2, and (e) O3 2*p* orbital resolved partial density of states (PDOS) in undoped Ba_2CaMoO_6 system.

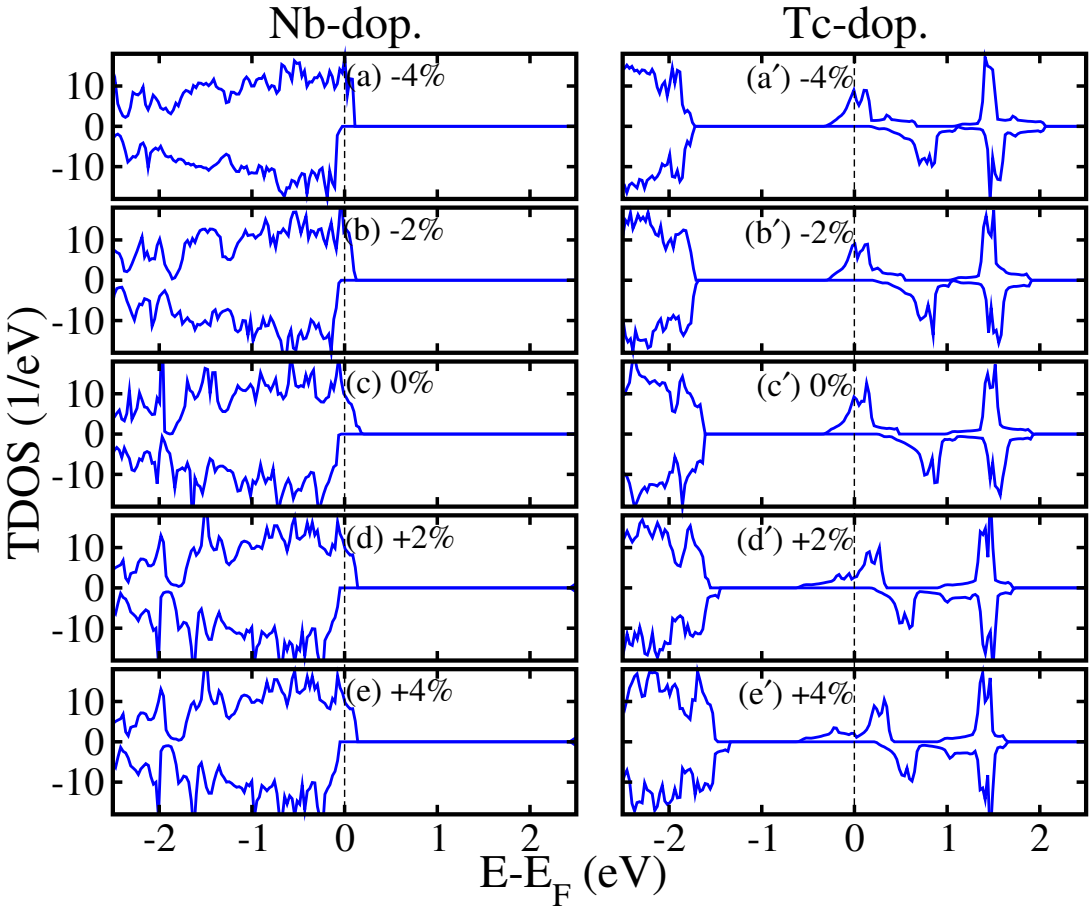

FIG. 2S: Calculated spin-polarized total density of states (TDOS) for (a/a′) −4%, (b/b′) −2%, (c/c′) 0% (unstrained), (d/d′) −2%, and (e/e′) +4% biaxial strains in Nb(left column)/Tc(right column)-doped Ba_2CaMO_6 systems. The "−" and "+" signs show compressive and tensile strains, respectively.