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Nb and Ta Layer Doping Effects on the Interfacial Energetics and Electronic Properties of $LaAlO_3/SrTiO_3$ Heterostructure: First-Principles Analysis

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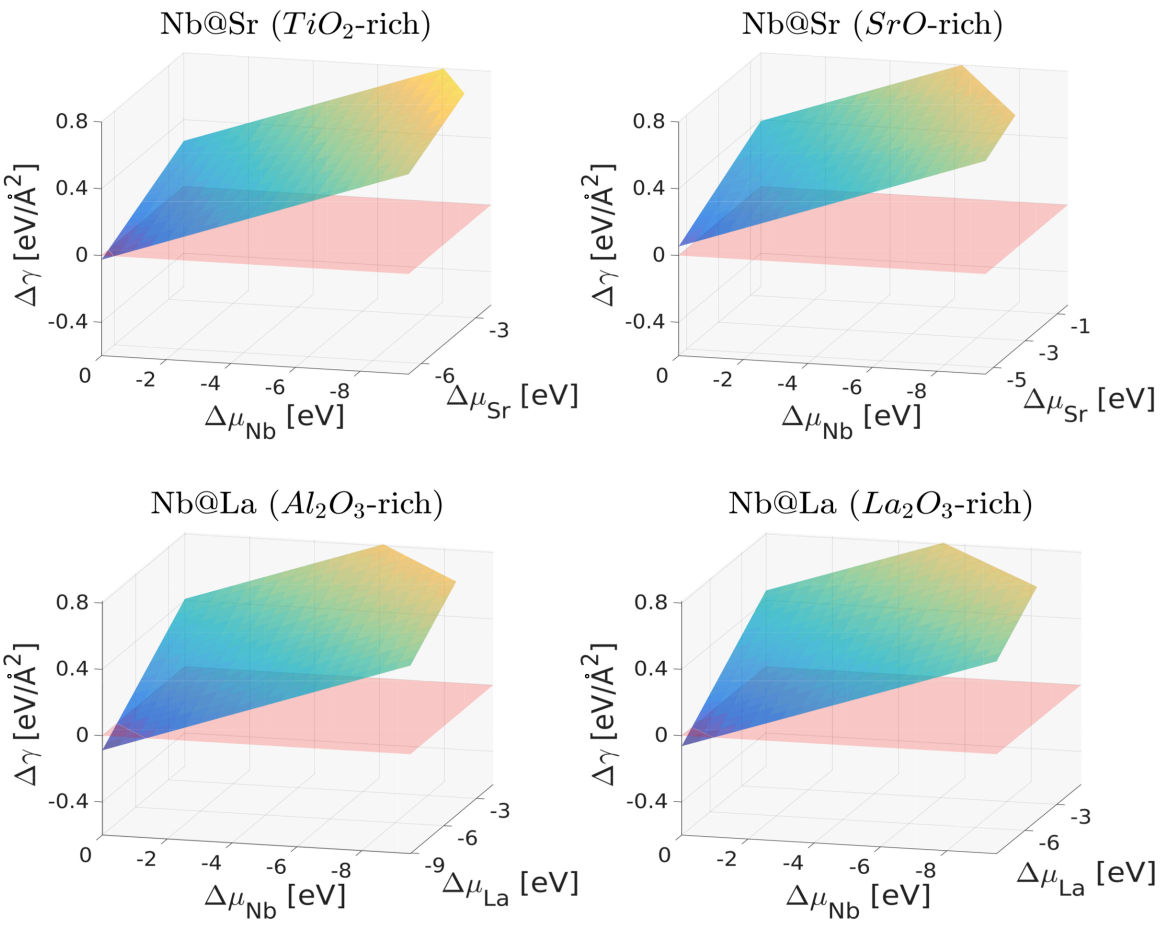

Figure 1S: Calculated change of interfacial energy between Nb@X (X=Sr and La) doped and the LAO/STO undoped HS systems. The Nb@Sr doping was considered under TiO_2 and SrO-rich conditions, respectively. The Nb@La doping was considered under Al_2O_3 and La_2O_3-rich conditions, respectively. The translucent red plane delineates $\Delta\gamma = 0$, the value below that means that doping is energetically favorable.

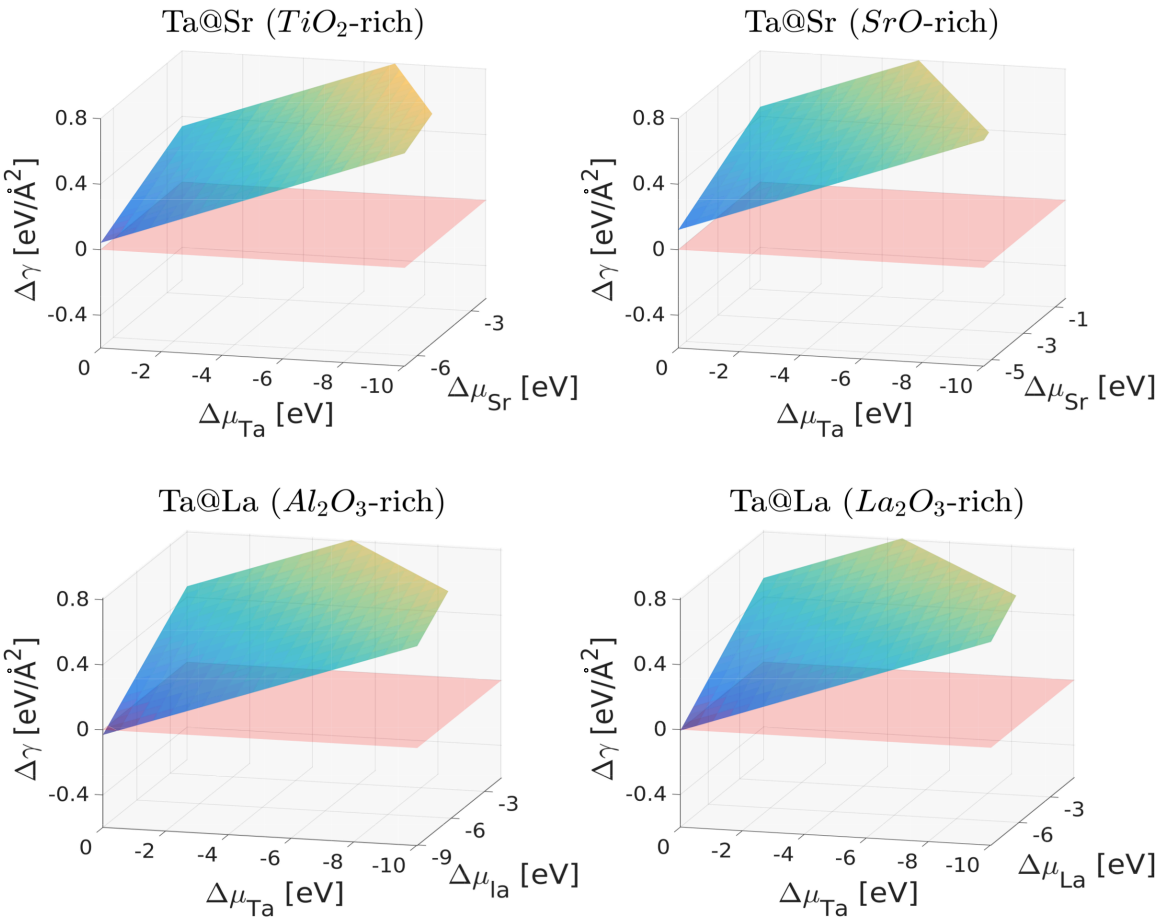

Figure 2S: Calculated change of interfacial energy between Ta@X (X=Sr and La) doped and the LAO/STO undoped HS systems.

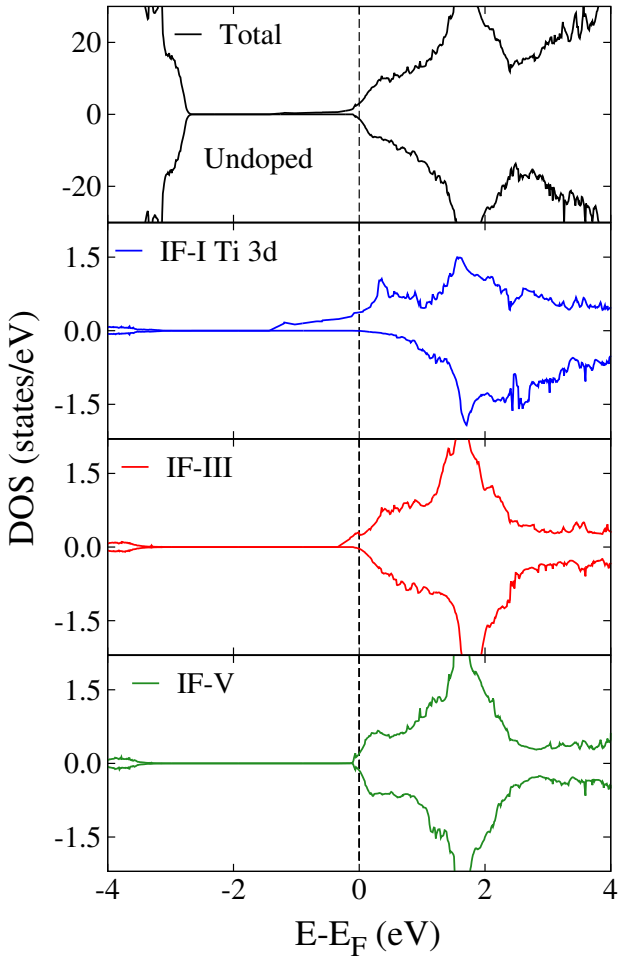

Figure 3S: Calculated spin-polarized total and Ti 3*d* partial DOS for undoped LAO/STO HS system. The IF-I, IF-III, and IF-V stand for the first, third, and fifth TiO_2 layers of STO near the interfacial region, respectively.