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

Electronic Supplemental Information

Thermodynamic stability of non-stoichiometric $SrFeO_{3-\delta}$: hybrid DFT study

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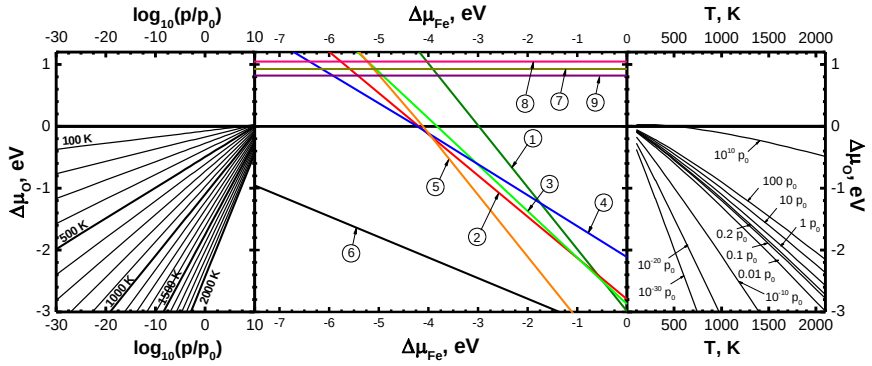
(a) ECP on Fe:



(b) All-electron Fe:

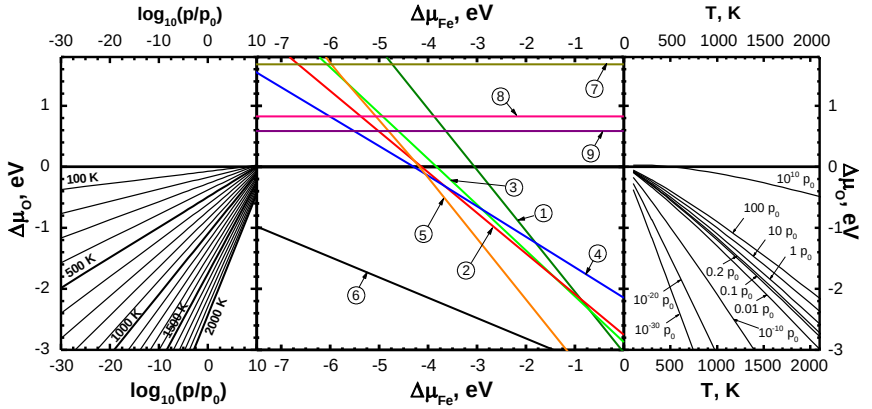
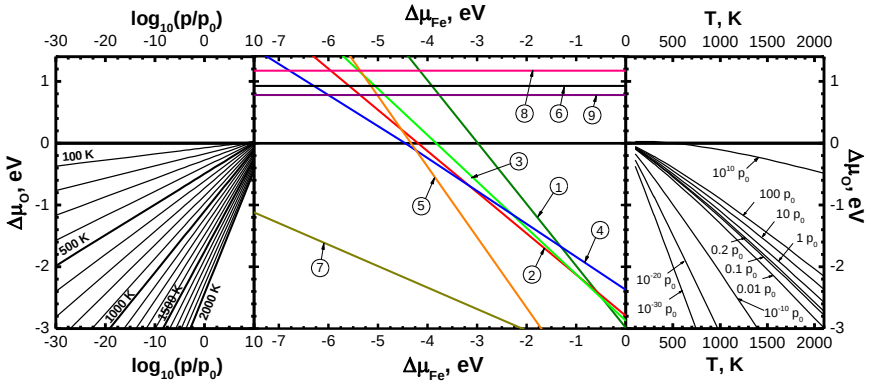


Figure S1. Phase diagrams for $SrFeO_3$: (a) based on Fe ECP treatment (b) based on Fe all electron treatment (c) based on experimental energies of formation. The energies of used to build these diagrams are provided in Table 7. The lines, pointed by numbers in circles describe conditions of forming of: (1) FeO, (2) Fe_2O_3, (3) Fe_3O_4, (4) SrO, (5) SrO_2, (6) Sr metal, (7) $SrFeO_{2.875}$, (8) $SrFeO_{2.75}$, (9) $SrFeO_{2.5}$. Side panels at (a,b) serve to convert values of oxygen chemical potential $\Delta\mu_O$ to easy observable values of T and oxygen partial pressure p_{O_2}.

(a) ECP on Fe:



(b) All-electron Fe:

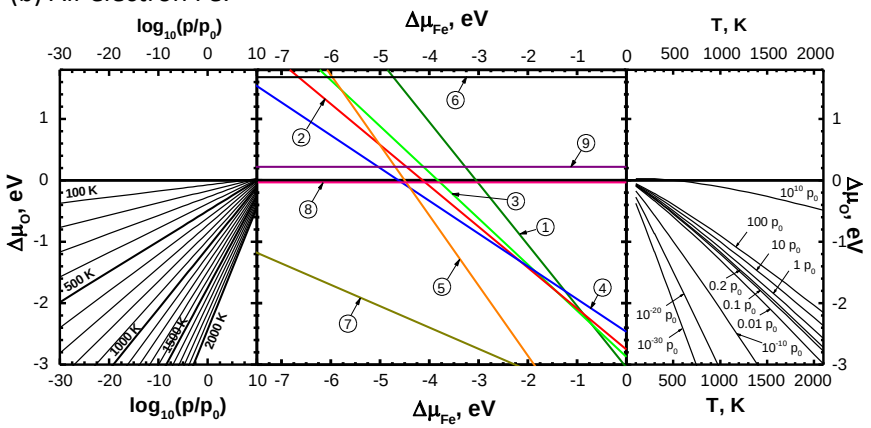
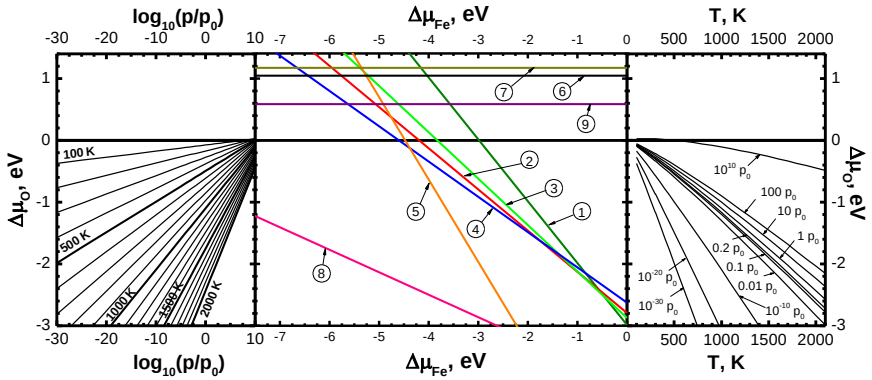


Figure S2. Phase diagrams for $SrFeO_{2.875}$: (a) based on Fe ECP treatment (b) based on Fe all electron treatment (c) based on experimental energies of formation. The energies of formation used to build these diagrams are provided in Tables 1 and 7. The lines, pointed by numbers in circles describe conditions of forming of: (1) FeO, (2) Fe_2O_3, (3) Fe_3O_4, (4) SrO, (5) SrO_2, (6) $SrFeO_3$, (7) Sr metal, (8) $SrFeO_{2.75}$, (9) $SrFeO_{2.5}$. Side panels at (a,b) serve to convert values of oxygen chemical potential $\Delta\mu_O$ to easy observable values of T and oxygen partial pressure p_{O_2}.

(a) ECP on Fe:



(b) All-electron Fe:

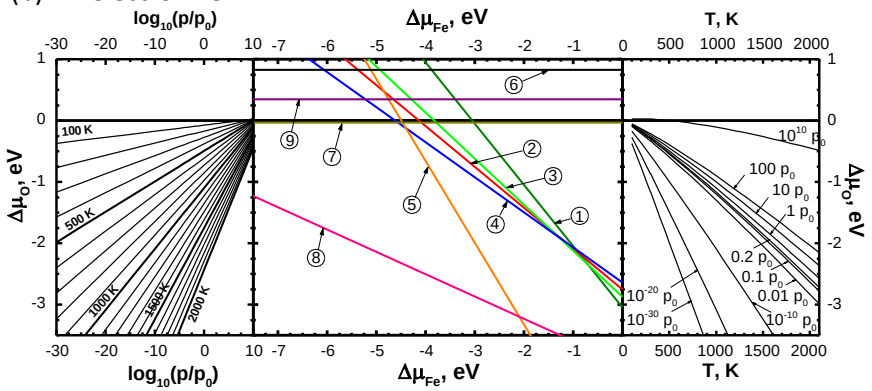


Figure S3. Phase diagrams for $SrFeO_{2.75}$: (a) based on Fe ECP treatment (b) based on Fe all electron treatment (c) based on experimental energies of formation. The energies of formation used to build these diagrams are provided in Tables 1 and 7. The lines, pointed by numbers in circles describe conditions of forming of: (1) FeO, (2) Fe_2O_3, (3) Fe_3O_4, (4) SrO, (5) SrO_2, (6) $SrFeO_3$, (7) $SrFeO_{2.875}$, (8) Sr metal, (9) $SrFeO_{2.5}$. Side panels at (a,b) serve to convert values of oxygen chemical potential $\Delta\mu_O$ to easy observable values of T and oxygen partial pressure p_{O_2}.