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Effects of oxygen pressure on morphology and surface energetics of β-PbO_2: Insight from DFT calculations

(Supplementary Information)

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A. The effect of spin-orbit coupling (SOC) on surface energies and Wulff construction

To understand the effect of spin-orbit coupling (SOC) on the surface energies, we performed test calculations of the surface energies which include SOC. It is found that SOC barely affects the surface energies and thereby the Wulff shapes as shown in Table S1 and Fig. S1.

Table S1 The calculated surface energies with and without spin-orbit coupling (SOC).

plane	surface energies (J/m^2)	
	PBEsol	PBEsol-SOC
110	0.72	0.72
100	0.82	0.83
101	1.03	1.02
001	1.33	1.31
111	1.44	1.42

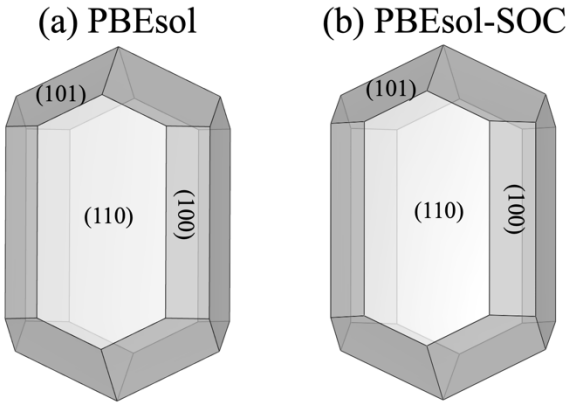

Figure S1. Thermodynamic equilibrium shape of stoichiometric β-PbO_2 obtained by the Wulff construction using (a) the PBEsol and (b) the PBEsol functional including spin-orbit coupling (SOC)

B. Formation enthalpies of metal oxides

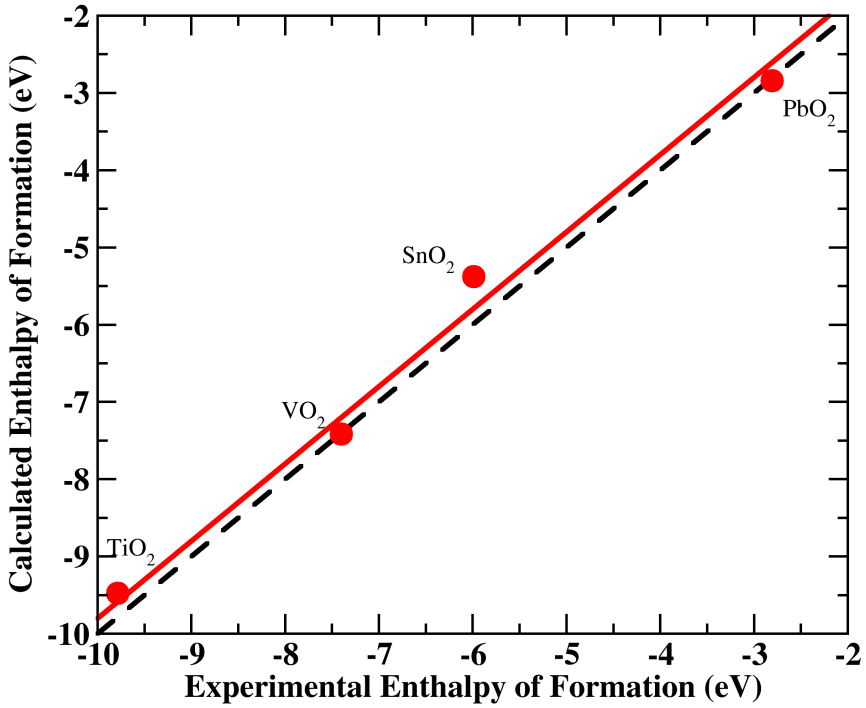

Figure S2. Calculated enthalpy of formation of selected metal oxides within the PBEsol functional as a function of experimental formation of enthalpy. The experimental values are taken from Ref. [1]

C. Atomic configurations of the non-stoichiometric surfaces

(110)

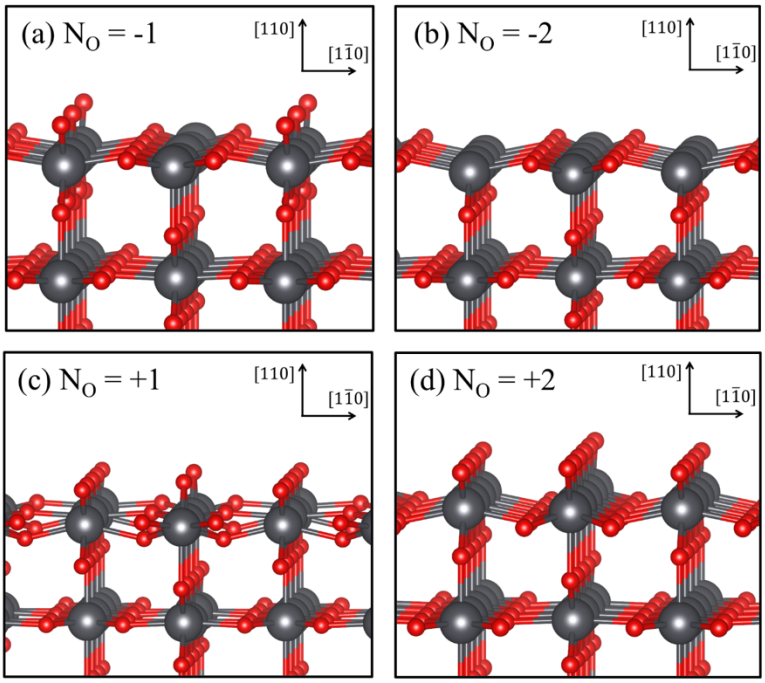

Figure S3. (110) surface with (a) N_O=-1, (b) N_O=-2, (c) N_O=+1, and (d) N_O=+2

(100)

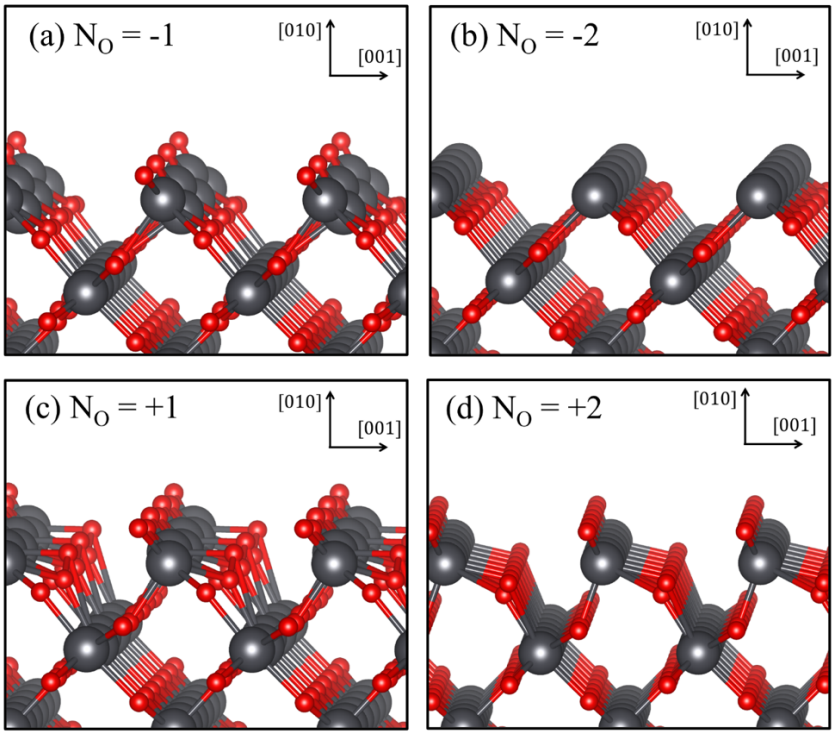

Figure S4. (100) surface with (a) N_O=-1, (b) N_O=-2, (c) N_O=+1, and (d) N_O=+2

(101)

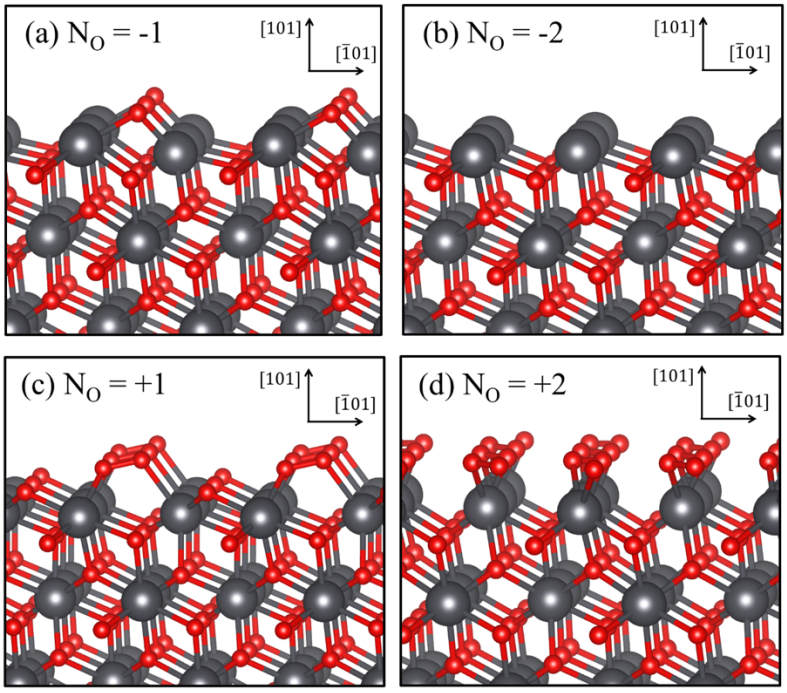

Figure S5. (101) surface with (a) N_O=-1, (b) N_O=-2, (c) N_O=+1, and (d) N_O=+2

(001)

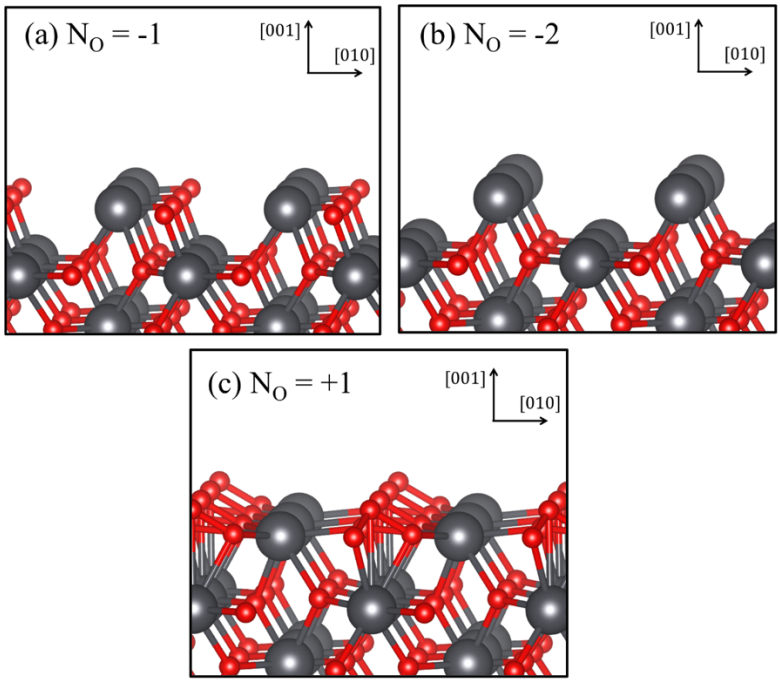

Figure S6. (001) surface with (a) N_O=-1, (b) N_O=-2, and (c) N_O=+1

(111)

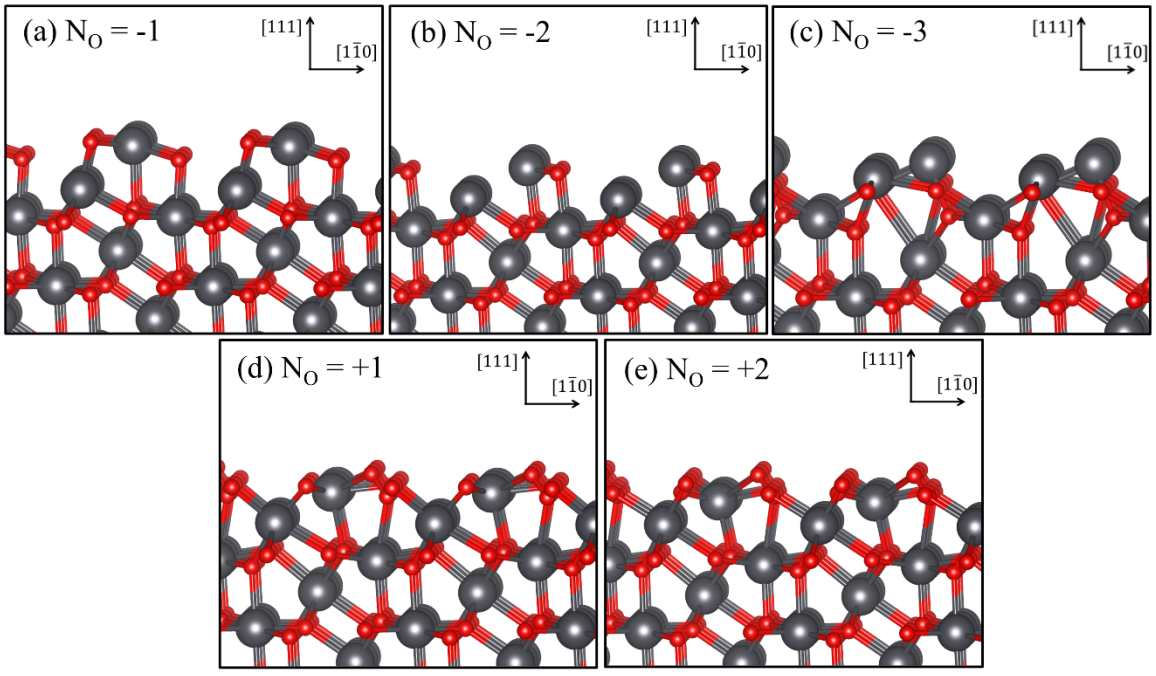

Figure S7 (111) surface with (a) N_O=-1, (b) N_O=-2, (c) N_O=-3, (d) N_O=+1, and(d) N_O=+2

References

[1] M. Binnewies and E. Milke, *Thermochemical data of elements and compounds*. (Wiley Online Library, 2002).