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

Supplementary Information for

High-throughput computational materials screening of transition metal peroxides

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Phase	Lattice Parameters (Å)	Atomic coordinates (fractional)
ScO_2 [$P2_1/c$]	a = 3.724, b =5.838, c =5.902 α =92.718, β = γ = 90.000	Sc 0.028 0.224 0.839 O1 0.460 0.859 0.317 O2 0.845 0.548 0.440
TiO_3 [$Pmmn$]	a = 2.948, b =3.948, c =7.113 α = β = γ = 90.000	Ti 0.000 0.500 0.350 O1 0.500 0.500 0.545 O2 0.000 0.184 0.818

Table S1. Detailed structural information of the ScO_2 and TiO_3.

Phase	Atom	Charge	$\sigma(e)$
ScO_2 [$P2_1/c$]	Sc	1.22	-1.78
	O1	7.16	1.16
	O2	6.62	0.62
TiO_3 [$Pmmn$]	Ti	2.12	-1.88
	O1	6.98	0.98
	O2	6.45	0.45

Table S2. Residual charges on metal and O atoms based on the Bader charge analysis in ScO_2 and TiO_3. The positive and negative values of σ represent the number of charges gained and lost by the atom.

The calculated formula for the convex hulls of formation enthalpy (ΔE_f)is defined as follows:

$$\Delta E_f(MO_x) = [E(MO_x) - E(M) - xE(O)] / (1+x), M=Sc, Ti$$

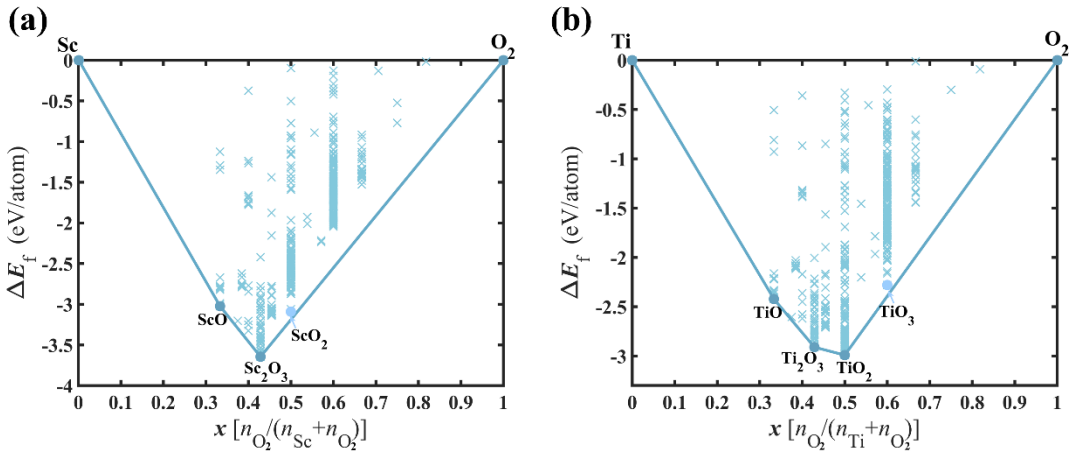

Fig. S1. (a), (b) The formation enthalpy of various Sc-O and Ti-O compounds.

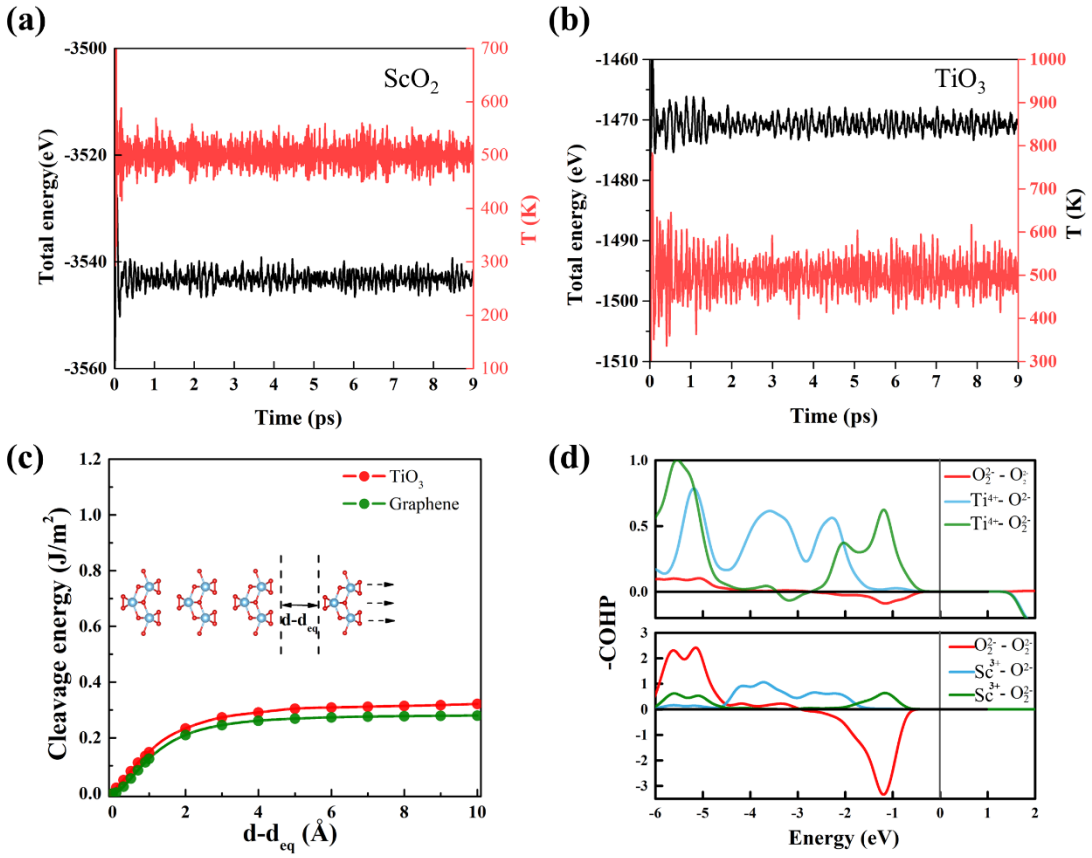

Fig. S2 (a), (b) Fluctuations of total energy and temperature with respect to AIMD steps at 500 K for ScO_2 and TiO_3. (c) Calculated cleavage energy of monolayer TiO_3 compared with the cleavage energy of monolayer graphene. (d) Negative crystal orbital Hamilton population (-COHP) of average $O^{2-}_2 - O^{2-}_2, Ti^{4+} - O^{2-}, Ti^{4+} - O^{2-}_2, Sc^{3+} - O^{2-}_2$ *and* $Sc^{3+} - O^{2-}$ bonds in the bulk ScO_2 and single layered TiO_3.

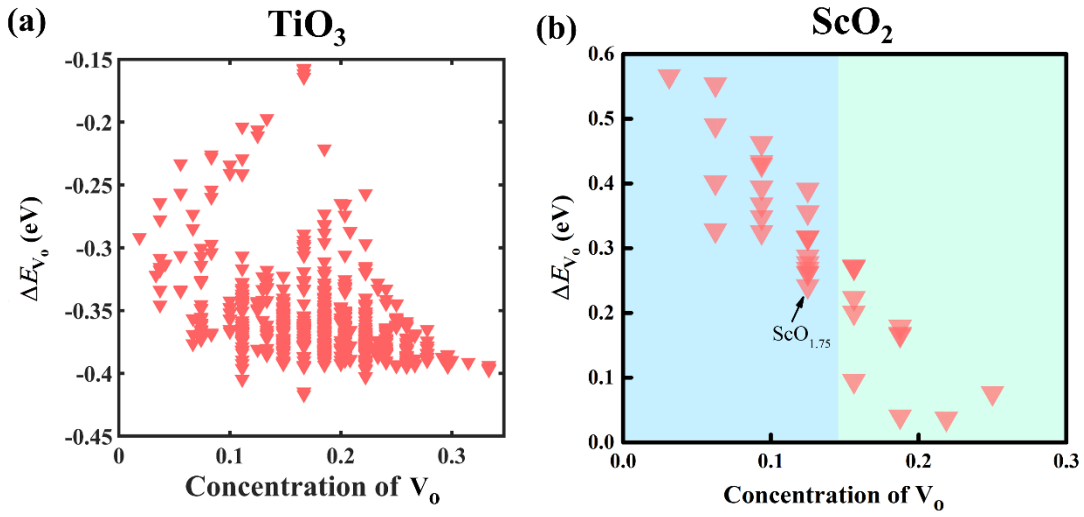

Fig. S3 (a) The average formation energy ΔE_{V_O} varies with oxygen vacancy concentration for the 2 $\times$ 2 $\times$ 1, $\sqrt{5} \times \sqrt{5} \times 1$, and 3 $\times$ 3 $\times$ 1 supercell of TiO_3. (b) The average formation energy ΔE_{V_O} varies with oxygen vacancy concentration for 2 $\times$ 2 $\times$ 1 supercell of ScO_2. The right part indicates that the defect structure exhibits a higher degree of distortion.