Influence of Ti vacancy defects on the dissolution of O-adsorbed Ti(0001) surface: A first-principles study

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■ **Table S1.** Overlap population of Ti-O systems under different θ.

θ (ML)	$D_{Ti\text{-}O}$ (Å)		$D_{O\text{-}O}$ (Å)		Population of Ti-O bond		Population of O-O bond	
	Ti(0001)/O	Ti(0001)/O-vac	Ti(0001)/O	Ti(0001)/O-vac	Ti(0001)/O	Ti(0001)/O-vac	Ti(0001)/O	Ti(0001)/O-vac
1/9	1.933	1.949	—	—	0.360	0.343	—	—
2/9	1.932	1.946	—	—	0.360	0.350	—	—
1/3	1.929	1.934	—	—	0.357	0.348	—	—
4/9	1.932	1.942	—	—	0.365	0.353	—	—
5/9	1.929	1.893	2.751	2.895	0.369	0.405	-0.020	-0.010
2/3	1.922	1.895	2.938	2.911	0.367	0.393	-0.010	-0.010
7/9	1.926	1.882	2.846	2.868	0.374	0.411	-0.016	-0.013
8/9	1.923	1.883	2.829	2.891	0.376	0.404	-0.018	-0.013
1	1.920	1.887	2.776	2.941	0.380	0.406	-0.020	-0.020

Notes: $D_{Ti\text{-}O}$ represents the average bond length of Ti-O, as shown in **Fig. 7(b)**. $D_{O\text{-}O}$ represents the average bond length of O-O.