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Electronic Supplementary Information (ESI)

Effect of Surface Defects on the Interaction of Oxygen Molecule with ZnO($10\bar{1}0$) Surface

Adhitya Gandaryus Saputro[1,2,3,*], Fiki Taufik Akbar[4], Nikita Pradnya Paramita Setyagar[1], Mohammad Kemal Agusta[1,2], Aditya Dimas Pramudya[5] and Hermawan Kresno Dipojono[1,2,]**

[1] Advanced Functional Materials Research Group, Institut Teknologi Bandung, Jl.Ganesha 10, Bandung 40132, Indonesia
[2] Research Center for Nanosciences and Nanotechnology, Institut Teknologi Bandung, Jl. Ganesha 10, Bandung 40132, Indonesia
[3] Engineering Physics Program, Institut Teknologi Sumatera (ITERA), Jl Terusan Ryacudu, Lampung 35365, Indonesia
[4] Theoretical High Energy Physics Research Group, Institut Teknologi Bandung, Jl.Ganesha 10, Bandung 40132, Indonesia
[5] Ecology Research Group, Institut Teknologi Bandung, Jl.Ganesha 10, Bandung 40132, Indonesia
Email: * ganda@tf.itb.ac.id, ** dipojono@tf.itb.ac.id

Effect of DFT+U correction and dispersion correction on the O_2 adsorption on ZnO($10\bar{1}0$) surface

The effect of the inclusion of DFT+U correction and dispersion correction to the O_2 adsorption energies and configurations on ZnO($10\bar{1}0$) surfaces are presented in Table S1. In general, we find that the inclusion of these parameters does not significantly affect the O_2 adsorption sites and their geometrical structures. However, this inclusion affects the value of adsorption energies. The inclusion of dispersion correction makes the calculated adsorption energy becomes more negative. We expect that the absence of the dispersion correction will not change the reaction pathway of the O_2 dissociation process, but it will lower the calculated dissociation energy since its inclusion makes the O_2 adsorption energy become stronger.

Table S1. Effect of DFT+U correction and dispersion correction on the adsorption geometries and adsorption energy of O_2 molecule on ZnO($10\bar{1}0$) surfaces.

	PBE + U, DFT-D2			PBE + U			PBE		
Surface	**Surface–O_2* (Å)**	**O–O* (Å)**	**E_{ads} (eV)**	**Surface–O_2* (Å)**	**O–O* (Å)**	**E_{ads} (eV)**	**Surface–O_2* (Å)**	**O–O* (Å)**	**E_{ads} (eV)**
Stoichiometric	2.454	1.23	-0.19	2.726	1.224	-0.06	2.603	1.226	-0.06
O vacancy	1.891	1.496	-2.08	1.893	1.495	-1.77	1.880	1.500	-1.77
Zn vacancy	1.598	1.233	-0.81	1.594	1.233	-0.60	1.657	1.230	-0.10
Zn-O vacancy	2.155	1.288	-0.55	2.180	1.282	-0.23	2.130	1.284	-0.33
Isolated O_2		1.222			1.222			1.222	

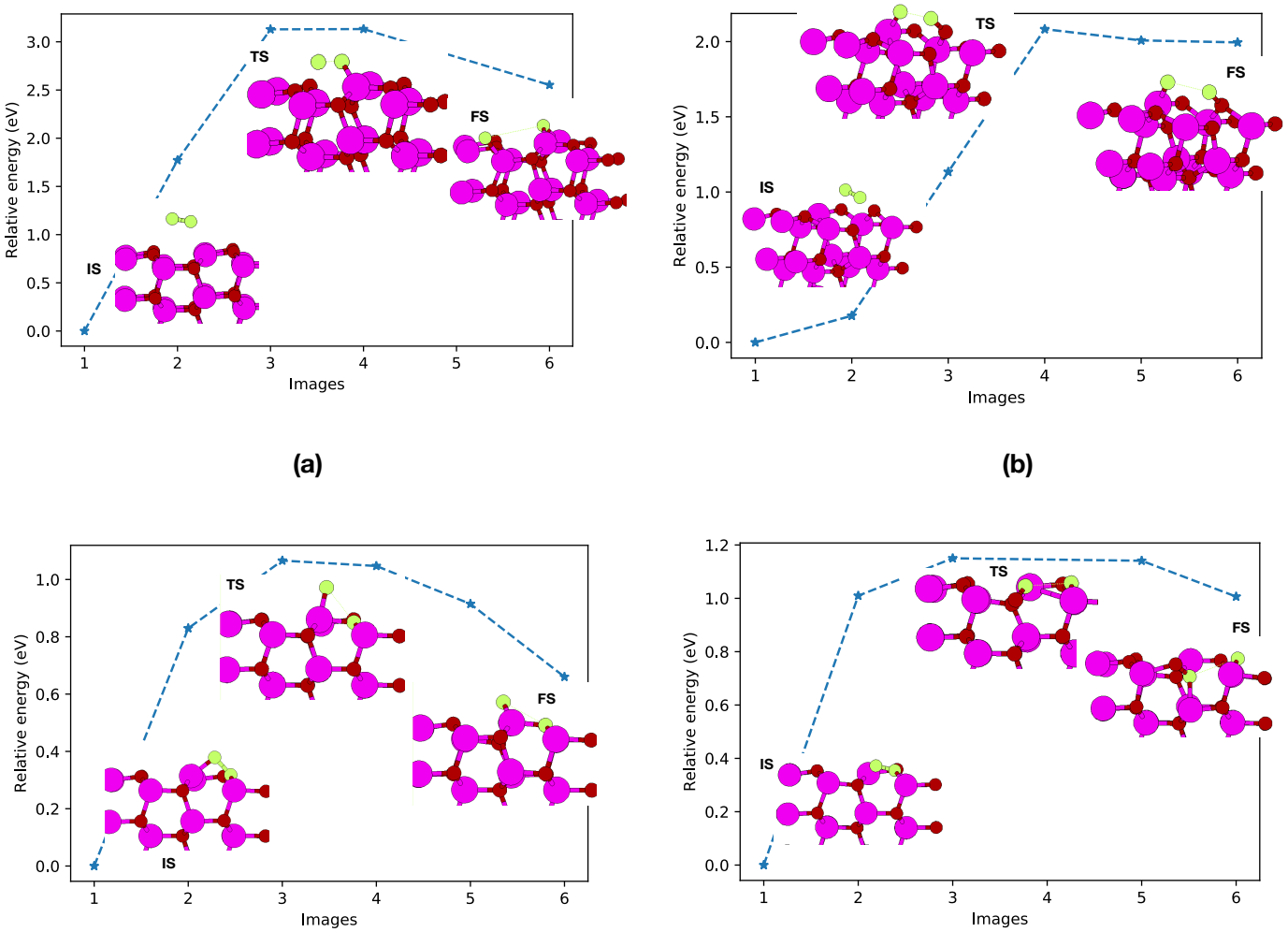

Figure S1. The minimum energy pathway (MEP) for O_2 dissociation on (a) stoichiometric ZnO($10\bar{1}0$) surface, (b) surface with Zn vacancy, (c) O vacancy, and (d) Zn-O dimer vacancy. IS, TS and FS correspond to initial state, transition state and final state, respectively.

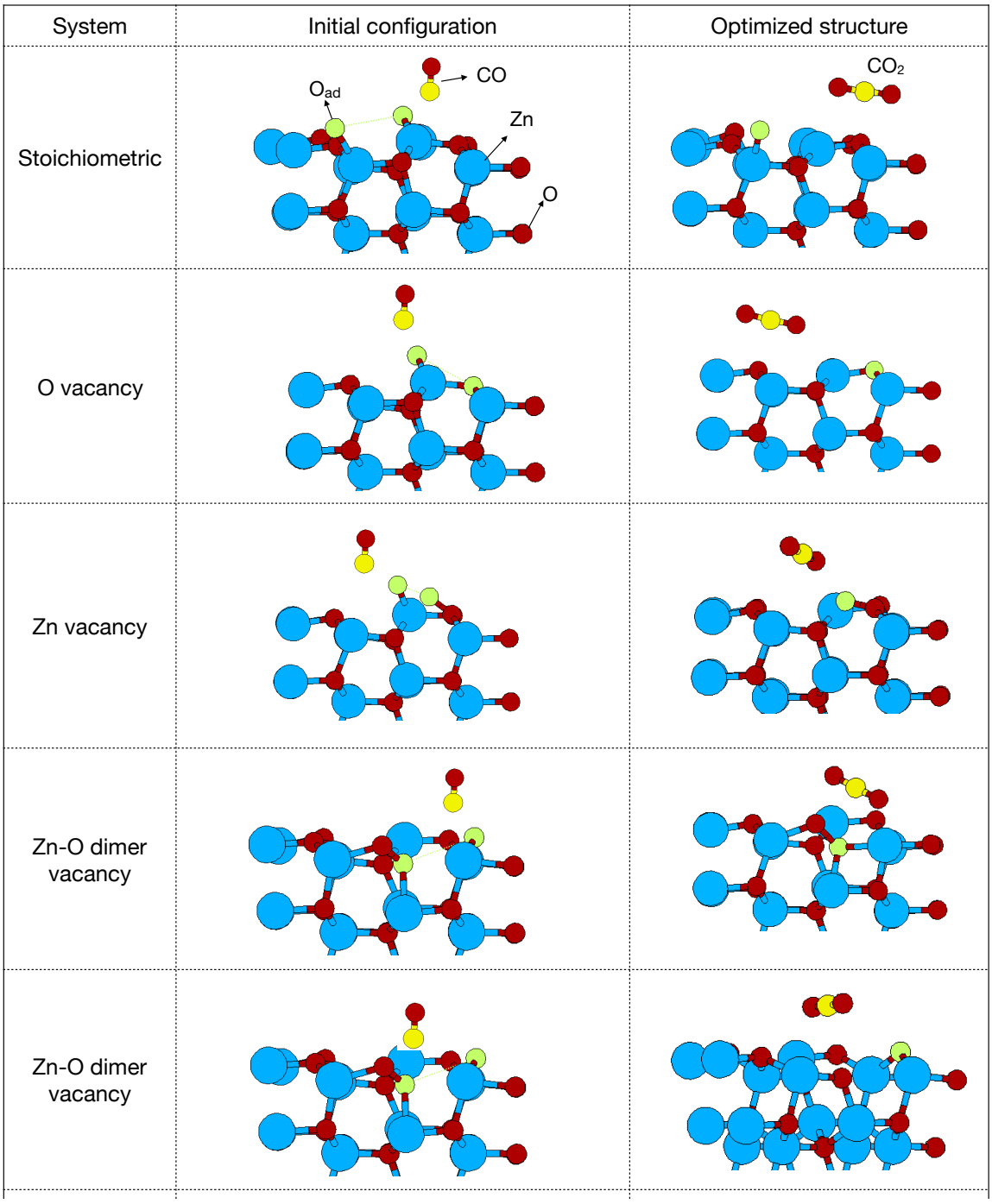

Figure S2. The initial and optimized structure of the interaction of CO molecule with the adsorbed atomic oxygen (O*) on ZnO($10\bar{1}0$) surfaces. This interaction spontaneously forms a CO_2 molecule for all surface configurations.