

Mitigation of CO poisoning on functionalized Pt/TiN surfaces

R. Q. Zhang^{1,2}, C.-E. Kim¹, B.-D. Yu³, C. Stampfl^{4,1}, and A. Soon^{1,4*}

¹*Department of Materials Science and Engineering, Yonsei University, 120-749, Seoul, Korea*

²*School of Chemical Engineering and Bioengineering, Washington State University, 99163, WA*

³*Department of Physics, University of Seoul, Seoul 130-743, Korea*

⁴*School of Physics, The University of Sydney, Sydney NSW 2006, Australia*

Table S1. The adsorption energy (with ZPE correction) for different atoms and molecular species adsorbed on the Pt/TiN(100) surface. The positive and negative values correspond to adsorption that is either endothermic or exothermic, respectively.

Adsorption energy (eV)	T_{Pt}	T_{Ti}	B_{Ti}
CO ₂	-0.19	*	*
CO	-1.24	-0.98	*
H	-0.43	*	0.17
H ₂	0.06	0.07	*
OH	0.13	-0.60	0.29
O ₂	-0.66	-2.30	*
O	-1.42	-2.64	-1.67

* notes that molecules on these sites are unstable (i.e. they do not bind on the surface).

* Corresponding author. E-mail: aloysius.soon@yonsei.ac.kr