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A DFT and KMC Based Study on the Mechanism of Water Gas Shift Reaction on Pd(100) Surface

Arunabhiram Chutia[1,2]*, Adam Thetford[2,3,4], Michail Stamatakis[5], C. Richard A. Catlow[2,4,6]*

[1]School of Chemistry, Brayford Pool, University of Lincoln, Lincoln, LN6 7TS United Kingdom

[2]UK Catalysis Hub, RCaH, Rutherford Appleton Laboratory, Didcot, OX11 OFA, United Kingdom

[3]Department of Chemistry, University of Manchester, United Kingdom

[4]Department of Chemistry, University College London, Gordon Street, London, WC1H 0AJ, United Kingdom

[5]Department of Chemical Engineering, University College London, Torrington Place, London, WC1E 7JE, United Kingdom

[6]Cardiff Catalysis Institute, School of Chemistry, Cardiff University, Cardiff, CF10 3AT, United Kingdom

Email: achutia@lincoln.ac.uk and c.r.a.catlow@ucl.ac.uk

Table S1. the interaction energies using DFT on two adjacent molecules (both for the same or for different species) on the same surface.

Adsorbed	Interaction energy
CO + O	0.196
CO + OH	0.107
OH + H	0.043
O + H	0.368
H_2O + O	0.354
H + H	0.077
(CO+ CO)bb	0.128
(CO+ CO) b4	0.103
(CO +CO) bt(bb)	0.067

Table S2. The energy barriers for the forward and reverse reactions and the $\Delta E_{reaction}$

Steps	eV		
	Ef	Er	$\Delta E_{reaction}$
1	1.320	0.240	1.080
2	0.880	1.410	-0.530
3	0.320	0.350	-0.030
4	0.810	0.018	0.792
5	0.690	0.439	0.251
6	0.720	1.471	-0.751
7	0.540	0.850	-0.310