Supplemental Data:

The influence of hydroxyls on Pd-atom mobility and clustering on rutile TiO_2(011)-2×1

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Table S1. Hydrogen adsorption energies bonds calculated with ReaxFF and DFT at varying sites and hydrogen coverages forming (OH) bonds on the TiO_2(011)-2x1 surface.

H-Adsorption Site	Coverage	ReaxFF E_{ads} (kcal mol^{-1})	DFT[a] E_{ads} (kcal mol^{-1})
atop	0.25	2.2	0.7
atop-atop	0.50	2.5	2.3
atop-atop (adjacent)	0.50	3.8	2.5
atop-bridge	0.50	5.2	7.8
atop-bridge (adjacent)	0.50	5.3	5.8
atop-bridge (adjacent)	0.50	6.1	6.9
bridge	0.25	8.4	11.3
trough	0.25	27.2	12.7
subsurface	0.25	20.7	11.1

a) Tao, J.; Cuan, Q.; Gong, X.-Q.; Batzill, M., *J. Phys. Chem. C* **2012**, 116 (38), 20438-20446.

Table S2. ReaxFF and DFT Adsorption Energies for Pd single atoms and clusters of varying size on the TiO_2(011)-2x1 surface.

Cluster Size	Site	ReaxFF E_{ads} (kcal mol^{-1})	DFT Eads (kcal mol^{-1})
Pd_1	hollow	-48.4	-50.7
Pd_1	trough	-48.2	-46.0
Pd_1	bridge-atop	-36.2	-33.3
Pd_1	bridge-trough	-47.9	-46.1
Pd_2	trough	-48.1	-45.4
Pd_3	hollow	-54.9	-52.0
Pd_4	hollow	-55.5	-54.4