SUPPORTING INFORMATION

Using Photoelectron Spectroscopy and Quantum Mechanics to Determine d-Band Energies of Metals for Catalytic Applications

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Table S1: Refinement parameters applied to the calculated DOS. "Shift" and "Stretch" refer to the offset and the slope of a linear recalibration of the energy axis (using the Fermi energy as the mathematical origin), respectively, and "t_{2g}", "e_g", "p", and "s" refer to the relative weights of the symmetry-resolved components.

Element	Shift (eV)	Stretch	t_{2g}	e_g	p	s
Fe	-0.1	0.90	1	1	1	1
Co	-0.2	0.76	1	1	1	1
Ni	-0.2	0.69	1	1.6	1	1
Cu	0.0	1.09	1	2.1	1	1
Pd	0.0	1.00	1	2.6	1	1
Ag	0.0	1.23	1	2.0	1	1
Pt	0.0	1.12	1	2.1	1	1

Au	0.0	1.14	1	2.6	1	1

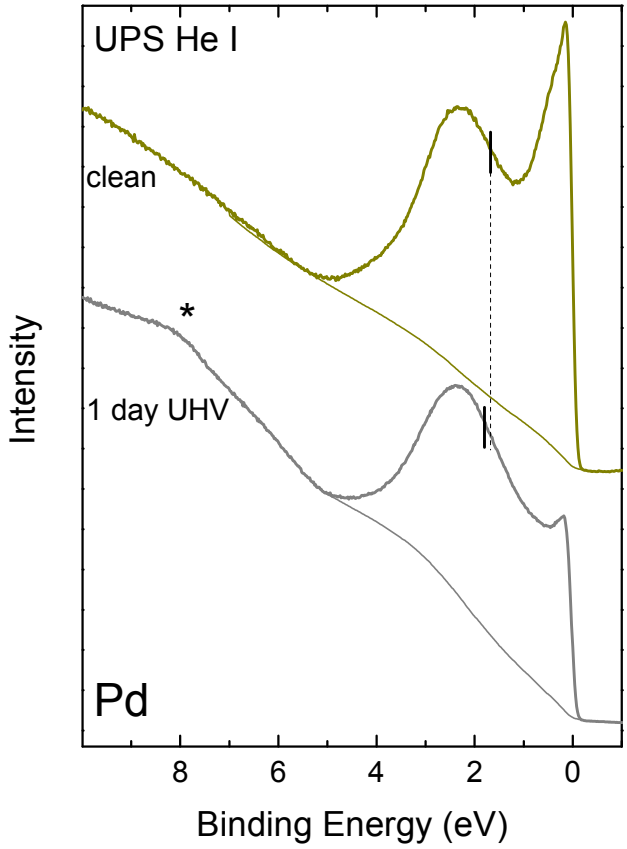

Fig. S1: UPS He I valence band spectra of a polycrystalline Pd foil immediately after Ar^+ sputtering (top) and after one day of storage in UHV (bottom). The adsorption of residual gases leads to a significant drop in intensity close to the Fermi energy, adsorbate states at higher binding energies (marked with a "*"), distinct changes in the background as indicated by a thin line underneath each spectrum, and a small change in the position of the d-band center (shown by the vertical solid and dashed lines).