

Supporting Information to:

**A unified study for water adsorption on metals:
meaningful models from structural motifs**

Guillem Revilla-López, Núria López*

*Institute of Chemical Research of Catalonia, ICIQ, Av. Països Catalans 16, 43007
Tarragona, Spain; nlopez@iciq.es*

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Figure S1. Convergence tests performed for adsorption energies, E_{ads} in eV/H₂O, on Pd(111) surface with increasing k-point densities (left) and kinetic cut-off energies Ice-like, sqrt(37) and Rosette (blue, green and red colors respectively).

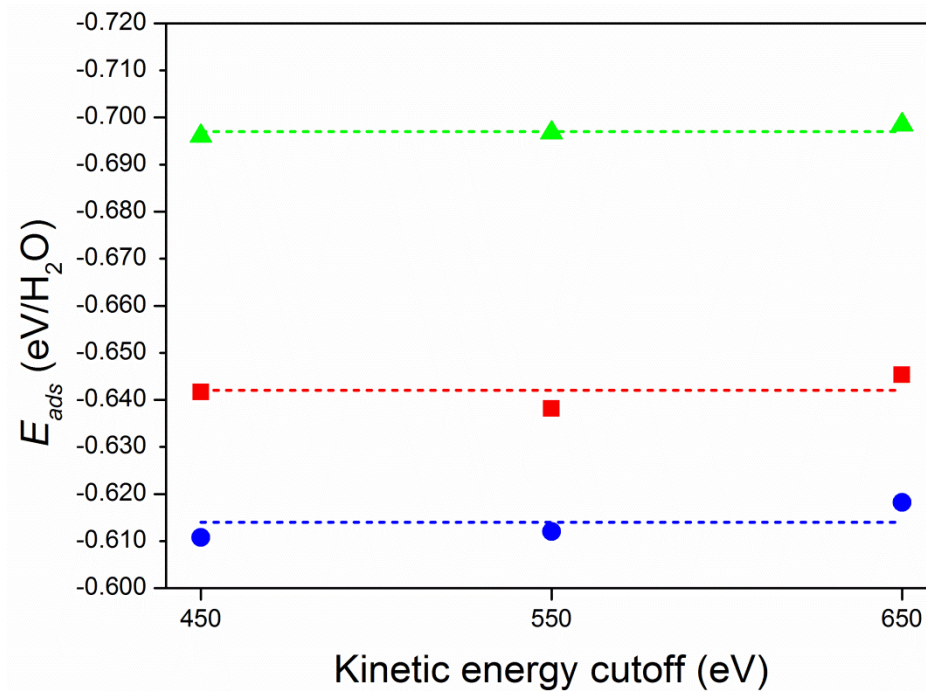
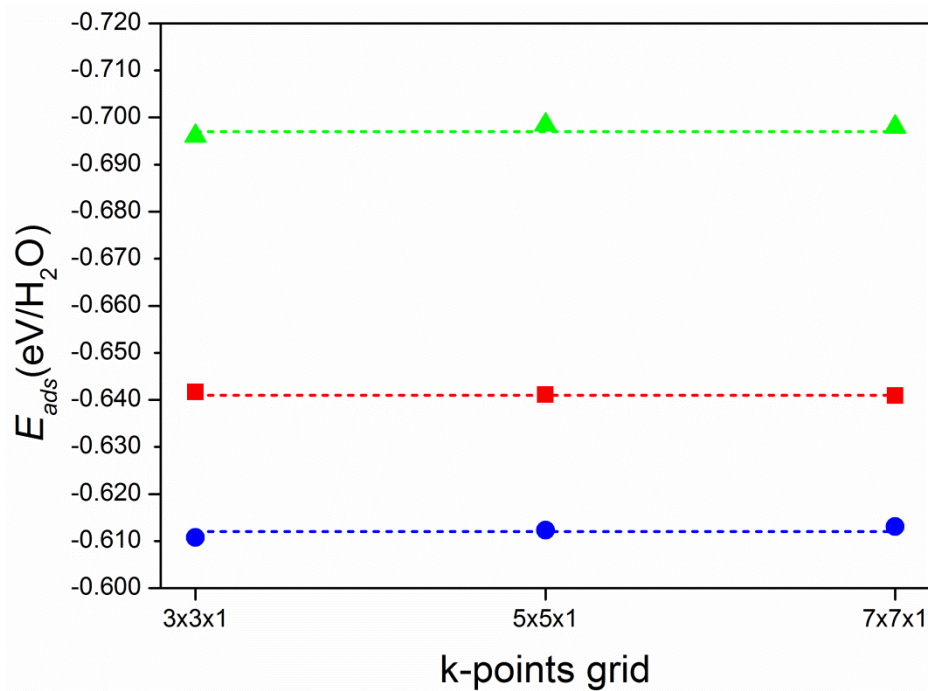


Table S1. Isolated water adsorption energy (in eV/H₂O), E_M^w for the unstrained (111) facets of metals in this work. Three different configurations are presented: flat, $E_M^{w,f}$; H-down, $E_M^{w,H}$, dissociated, $E_M^{w,d}$. Energies are in eV/H₂O.

	$E_M^{w,f}$	$E_M^{w,H}$	$E_M^{w,d}$	$E_M^{w,V}$
Pd(111)	-0.367	-0.130	N.A.	-0.405
Pt(111)	-0.344	-0.120	N.A.	-0.084
Ru(0001)	-0.490	-0.144	-0.836	N.A.
Ir(111)	-0.395	-0.154	N.A.	N.A.
Rh(111)	-0.443	-0.166	-0.334	N.A.
Au(111)	-0.217	-0.106	N.A.	N.A.
Ag(111)	-0.268	-0.114	N.A.	N.A.