Abstract Submitted
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Water films on transition metal surfaces: A physical disclosure of adsorption energy[1] GUILLEM REVILLA-LÓPEZ, NURIA LÓPEZ, Institute of Chemical Research of Catalonia, ICIQ, Av. Països Catalans 16, 43007 Tarragona, THEORETICAL HETEROGENEOUS CATALYSIS GROUP TEAM — Our work reports novel physical models derived from DFT calculations including van der Waals forces for the adsorption of different water motifs: ice bilayer, $\sqrt{37}$ x$\sqrt{37}$-R 25.3° and rosette on transition metal surfaces. This energy decomposition scheme is obtained by analyzing the two driving energies of adsorption: water-water and water-metal interactions. The former explained by single water adsorption and the latter by ice resonance stabilization. These two magnitudes drive, to different extent, the adsorption of ice bilayer and $\sqrt{37}$ whereas rosette motif lacks the resonance contribution. The equations successfully reproduce and predict the experimental results for the wettability and the dissociation of water films on the fcc(111) and hcp(0001) facets of Pd, Pt, Ru Ir, Rh, Au, and Ag. So happens for the temperature of the hydrophobic/hydrophilic water film transition and for the effect of the surface roughness on it. Furthermore, the metastability and the wettability of other water films like $\sqrt{39}$ x$\sqrt{39}$-R 16.1° can be anticipated by the rationalization of their geometry and their dissociation state.

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