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Insight into water molecules bonding on 4d metal surfaces JAVIER CARRASCO, Fritz-Haber-Institut der Max-Planck-Gesellschaft, Faradayweg 4-6, 14195, Berlin, Germany, ANGELOS MICHAELIDES, MATTHIAS SCHEFFLER — Water-metal interactions are of capital importance to a wide variety of phenomena in materials science, catalysis, corrosion, electrochemistry, etc. Here we address the nature of the bond between water molecules and metal surfaces through a careful systematic study. Specifically, the bonding of isolated water molecules to a series of close-packed transition metal surfaces - Ru(0001), Rh(111), Pd(111) and Ag(111) - has been examined in detail with density functional theory (DFT). Aiming to understand the origin behind energetic and structural trends along the 4d series we employ a range of analysis tools, such as decomposition of the density of states, electron density differences, electronic reactivity function and inspection of individual Kohn-Sham orbitals. The results obtained allow us to rationalize the bonding between water and transition metal surfaces as a balance of covalent and electrostatic interactions. A frontier orbital scheme based on so-called two-center four-electron interactions between molecular orbitals of water and d band states of the surface proves incisive in understanding these systems.

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