

Properties of metal-liquid interfaces derived from first principles

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Nowadays, electronic structure calculations based on density functional theory combine numerical efficiency with a sufficient accuracy to allow reliable predictions about properties of complex metal-liquid interfaces. I will first briefly summarize the factors underlying the reactivity of (bi-)metallic electrode surfaces made of transition metals (see, e.g., [1, 2]). I will then address the geometric and electronic structure of metal-water interfaces based on *ab initio* molecular dynamics simulations at room temperature [3]. At the more strongly interacting transition metal surfaces such as Pt and Ru, the simulations suggest that the hexagonal ordered structure might persist at room temperature, however, the orientation of the single water molecules is strongly fluctuating. Water layers have only a minor influence on the electronic structure of metallic electrodes and thus on the chemisorption strength in specific adsorption. Still, because of their large dipole moment and strong polarization, water layers lead to a significant work function change of metal electrodes. This translates into a close relation between the structure of the water layer and the electrode potential.

References

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