Computational Studies of the Electronic and Atomic Structure of Passivation Layers on Transition Metals

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With the development of self consistent tight binding methods, study of electrochemical interfaces by direct dynamics, in which electronic structure is followed adiabatically as atoms move, is becoming feasible for systems large enough to provide information useful to electrochemists. We report studies of the water/rutile, water/RuO_2, and titanium-metal/oxide interfaces, as well as studies or anatase and rutile nanoparticles in water which illustrate this point.