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Interaction of prophyrins with low coordinated sites on the MgO(001) surface OSMAN BARIS MALCIOGLU, MICHEL BOCKSTEDTE, Solid State Physics, FAU Erlangen-Nrnberg, Erlangen Germany — The functionalization of metal oxide surfaces with porphyrins is achieved via site selective linker groups and a specific metal center in the macrocycle. Metal oxide surfaces like MgO(001) have got a rather inert prestine surface and reactive low coordinated sites such as steps and kink-sites. Recently the metallization of H2TPP with Mg via low coordinated sites on MgO(001) has been demonstrated. The underlying mechanisms, however, remain unclear. Here we address this issue. We study the adsorption of H2TPP on MgO(001) and its interaction with low coordinated sites employing ab initio molecular dyanmics simulations. We find that H2TPP is mobile on the surface due to steric hindrance from phenyl rings preventing physisorption of the macrocycle, until a step or kink site is encountered. Upon encountering such a site, H2TPP anchors itself to form a rather stable complex, and spontaneously deprotonates from the macrocycle. We discuss the electronic and structural properties of the adsorbate complex, the intermediate and the metallized porphyrins using (hybrid) TDDFT and many body perturbation theory, identifying various effects that can be used to uniquely identify presence of such complexes.

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