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Electron Traps at the Ice Surface MICHEL BOCKSTEDTE, PHILIPP AUBURGER, ANJA MICHL, Theor. Festkoerperphysik, FAU Erlangen-Nuernberg, Erlangen, Germany — Water, water clusters and ice possess the fascinating ability to solvate electrons. On the surface of water cluster[1] and thin crystalline ice structures on a metal substrate[2] long-living solvated electron states were observed that evolve from pre-existing surface traps. The identification of such traps provides important insight into the electronic structure of the water or ice surface, and the dissociative interaction of electrons with adsorbates. Models[2,3] based on the bilayer terminated Ih-(0001) surface related such traps to orientational defects or vacancies. So far, the understanding of the electronic structure of the ice surface with the electron traps is incomplete. Here we address this issue including also water ad-structures[4] within hybrid density functional theory and many-body perturbation theory (G_0W_0). We identify a hierachy of traps with increasing vertical electron affinity, ranging from hexagon adrows to clusters of orientational defects and vacancies with dangling OH-groups.

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