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Covalent functionalization of ZnO nanowires ANDREIA LUISA DA ROSA, NEY MOREIRA, ADRIEL GARCIA, THOMAS FRAUENHEIM, University of Bremen — Understanding the interaction of organic species with inorganic nanostructures constitutes a step forward in the development of semiconductor based biosensors. In this work we have used density functional theory to investigate ZnO-(1010) nanowire surfaces modified with substituted methane molecules (Me-X, with X= OH, NH2, SH, COOH, and CN). We have found three relevant stabilization mechanisms acting on the surface stabilization: passivation of surface oxygen lone-pairs via dissociative chemisorption processes, electrostatic adsorbate-interations involving Zn surface sites and hydrogen bonding interactions involving oxygen surface sites. Covalent adsorbate-substrate interactions were found to play only a marginal role on the surface stabilization. Contradicting the usual chemical intuition, we have found no significant evidence for the formation of classical Lewis acid-base adducts on Zn surface sites. Finally we suggest that the functionalization with Me-COOH is also expected to be stable under ordinary laboratory conditions or in aqueous media.

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