

MAR06-2005-003833

Abstract for an Invited Paper
for the MAR06 Meeting of
the American Physical Society

Ab-initio simulations of H₂O interaction with b-SiC surfaces.

GIANCARLO CICERO, Politecnico of Turin

We report on the interaction of gas phase water molecules with polar and non polar stoichiometric surfaces of cubic silicon carbide, a leading candidate semiconductor for bio-compatible devices. Finite temperature ab-initio molecular dynamics shows that the specific geometric arrangement of atoms on the outermost surface layer is responsible for water orientation and coordination and thus plays a major role in determining the surface reactivity. In particular, irrespective of coverage, water spontaneously dissociates on both polar[1] Si-terminated (001) and non-polar[2] (110) surfaces, while the C-terminated (001) surface is non-reactive and hydrophobic. Based on our results, we propose that STM images and photoemission experiments may detect specific changes induced by water on both the structural and electronic properties of SiC surfaces. We completed our investigation by studying a realistic solid/liquid interface[3] for the case of Si-SiC(001), after full hydroxylation takes place. We observed the formation of a thin (≈ 3 Å) interfacial layer, which presents a higher density than bulk water. The liquid does not uniformly wet the surface, rather molecules preferably bind along directions parallel to the Si dimer rows. Our calculations also predict that at ≈ 1 nm, the structural and electronic properties of liquid water are weakly affected by one-dimensional confinement between hydrophilic, solid substrates. [1] G. Cicero, A. Catellani and G. Galli Phys Rev. Lett. 93 (2004), 0161102; G. Cicero, A. Catellani and G. Galli J. Phys. Chem. B 108 (2004), 16518. [2] A. Catellani, G. Cicero and G. Galli J. Chem. Phys., in press. [3] G. Cicero, J. Grossman, A. Catellani and G. Galli J. Am. Chem. Soc. 127 (2005), 6830.