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Towards SiC surface functionalization: an ab initio study ALESSANDRA CATELLANI, GIANCARLO CICERO, LLNL, CNR-IMEM TEAM, LLNL TEAM — We present a microscopic model of the interaction and adsorption mechanism of simple organic molecules on SiC surfaces as obtained from ab initio molecular dynamics simulations. Our results for the silicon terminated SiC(001) surface show that at variance with the most exploited semiconductors such as Si and GaAs, the most common functional groups chemisorb to the surface, as a consequence of the substrate polarity with exothermal reactions. The preferential chemisorption of thiolates in particular can lead to the realization of stable self-assembled monolayers, with no requirement of preliminar metallic deposition. Our results open the way to functionalization of silicon carbide, a leading candidate material for bio-compatible devices. Part of this work was performed under the auspices of the U.S. Department of Energy by University of California Lawrence Livermore National Laboratory under contract No. W-7405-Eng-48.

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