O 22: Invited Talk Johannes Pollmann

Time: Tuesday 10:15–11:00 Location: HE 101

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Adsorption Processes on SiC Surfaces: First-Principles Theory — •Johannes Pollmann — Institut für Festkörpertheorie, Universität Münster

The surface atomic structure, the topology of surface dangling bonds, and the high directionality of adsorbate-substrate interactions play a crucial role in the chemical activity of semiconductor surfaces. This has been well appreciated in many adsorption studies using silicon surfaces as prototype substrates. In this respect, the ionic compound semiconductor SiC offers particularly interesting new degrees of freedom because of its comparatively small lattice constant and its rich variety of surface reconstructions which give rise to very amazing and unusual adsorption processes in certain cases, as observed in experiment. For example, atomic hydrogen adsorbed on the fairly open SiC(001)-(3×2) surface does not lead to surface passivation but induces surface metallization. Likewise, molecular hydrogen readily adsorbes at room temperature dissociatively on the SiC(001)-c(4×2) surface while it does not react with SiC(001)-(3×2) although both surfaces are characterized by similar surface dimers. Interestingly, adsorption of hydrocarbons on SiC(001)-(3×2) versus Si(001)-(2×1) shows salient substrate-related differences, as well. In this talk adsorption of atomic and molecular hydrogen, acetylene, ethylene and benzene, as well as silicon-oxynitride adlayers on SiC surfaces will be discussed. Scrutinizing a number of reaction scenarios within first-principles theory allows us to identify the physical origin and nature of the peculiar adsorption behaviour of SiC surfaces.