

O 50: Invited Talk (Mahbube Hortamani)

Time: Thursday 14:00–14:45

Location: HSZ 02

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Si-based spintronics from first principles — MAHBUBE HORTAMANI — Max Planck Institute of Microstructure Physics — Fritz-Haber-Institut der Max-Planck-Gesellschaft

An important step is implementation of spin-based electronic functionality in Silicon devices. Remarkable progress made during the last two years [1] gives confidence that this is within reach, although significant challenges still remain. For example Si-based magnetic materials with a transition temperature higher than room temperature do not exist yet.

Here we discuss the specific aspects associated with ferromagnetic MnSi films on the Si substrate and determine how the electronic struc-

ture and the magnetic properties of these films and Silicon conspire to render a magnetic Si-based heterojunction.

Atomic-level insight is a necessary prerequisite to understand the mechanisms of basic physical processes such as surface diffusion and epitaxial growth. These processes are probed within the framework of density functional theory. Magnetic interactions of MnSi films at finite temperature are studied by means of a Heisenberg model. We predict the formation of a thin ferromagnetic film of MnSi in B2 (cesium chloride) crystal structure on the Si(001) surface with a Curie temperature around room temperature .

[1] Ian Appelbaum, B.Q. Huang, and D.J. Monsma, *Nature* 447, 295 (2007)