

Institut für Physik Physikalisches Kolloquium



Mittwoch, 07.11.2018, um 16:00 Uhr Ort: Reichenhainer Str. 90; Zentrales Hörsaal- und Seminargebäude, Raum 2/N013

Dr. Dirk König

Head of Research, Integrated Materials Design Centre (IMDC) node, University of New South Wales (UNSW), Sydney, Australia

Silicon Electronic Structure Modification: Beyond Impurity Doping

Impurity doping of silicon (Si) nano-volumes (NVs) as currently used in very large scale integration (VLSI) faces serious challenges at miniaturization efforts below the 14 nm technology node. Dopant out-diffusion, local density fluctuations and inactivation by clustering are major issues for Si field effect transistors (FETs). Self-purification and a massive increase in ionization energy cause doping to fail at Si nanocrystals (NCs) within the range of quantum confinement [1].

In analogy to modulation doping of III-V compounds [2], I demonstrate *direct* modulation doping for silicon [3] from SiO₂. By relocating the dopants from silicon to silicon dioxide, mentioned Si nanoscale doping problems are circumvented. In addition, the method provides excellent passivated hole-selective tunnelling contacts as required for high-efficiency Si solar cells. By screening suitable group IIIA and IIIB elements with theoretical and experimental methods, I will show that the choice of modulation acceptor is not trivial; knowledge of acceptors in bulk Si is inapplicable to SiO₂ modulation doping. Our findings demonstrate that several modulation acceptors exist, offering a tuning of hole-selective contacts for Si solar cells and tunnel-FETs. I will elucidate atomistic and quantum-chemical parameters which decide over acceptor candidates to work in SiO₂.

Ideally, n- or p-type conductivity in VLSI-Si requires just energy offsets of lowest unoccupied states (LUS) and of highest occupied states (HOS) between different regions of the same VLSI-Si volume. As a result, doping would be eliminated altogether. I will show in theory and experiment [4-6] that a few MLs of SiO_2 vs. Si_3N_4 achieve such an energy offset. The induced n- vs. p-type behaviour in VLSI-Si can potentially be big enough to allow for band-to-band tunnelling (BTBT) for realizing extremely small and fast tunnel-FETs. The maximum Si system size where this energy offset is substantial – nanocrystal, nanowire or nanowell – will be shown as a function of interface faceting and nanostructure shape [7].

- [1] Sci. Rep. 5, 09702 (2015)
- [2] Appl. Phys. Lett. **33**, 665 (1978)
- [3] Sci. Rep. **7**, 46703 (2017)
- [4] Phys. Rev. B 78, 035339 (2008)
- [5] Adv. Mater. Interfaces 1, 201400359 (2014)
- [6] Beilstein J. Nanotech, in print (2018)
- [7] AIP Adv. **6**, 085306 (2016)

Alle Zuhörer sind ab 15:45 zu Kaffee und Tee vor dem Hörsaal eingeladen.

