Sonderforschungsbereich 1277

Emergent Relativistic Effects in Condensed Matter -
From Fundamental Aspects to Electronic Functionality

SFB – Colloquium

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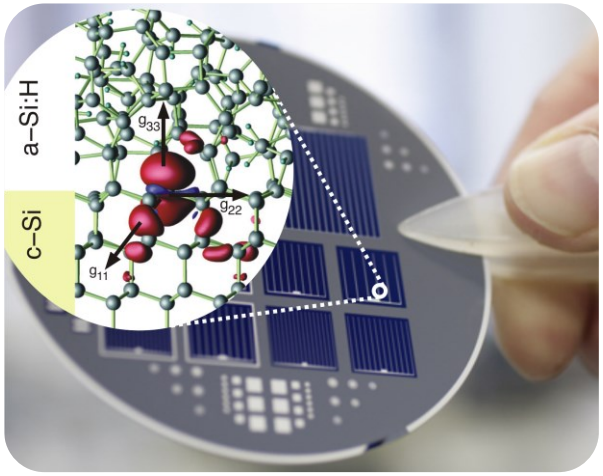
Date: Tuesday, 13 December 2023, 14:15, H34

Topic: Relativistic effects in solar cells – exploring spin-orbit coupling in the active interface of working devices

Abstract:

In the usual textbook view, relativistic effects are believed to be restricted to particles with a velocity comparable with the speed of light or to heavy atoms. However, spin-orbit coupling (SOC) can be significantly enhanced by structural inhomogeneities at surfaces and interfaces, where SOC triggers the precession of spins in modern spintronic devices via the Rashba effect. Furthermore, for the accurate simulation of spectroscopic data, SOC cannot be neglected in many cases, e.g. in magnetic resonance [1] or X-ray magnetic circular dichroism (XMCD) [2]. In this talk, an efficient full-relativistic approach is presented, which in the framework of density-functional theory (DFT) can be applied to systems with several hundreds of atoms, from nanoparticles, nanowires and surfaces to active interfaces of working devices like solar cells. Here, SOC is e.g. shown to determine the magnetic fingerprint of the charge carriers being separated at the (a-Si:H/c-Si) interface [3].



[1] Gerstmann *et al*., Phys. Rev. B **89**, 165431 (2014).
[2] Bouldi *et al*., Phys. Rev. B **196**, 240 (2019).
[3] George *et al*., Phys. Rev. Lett. **110**, 136803 (2013).

Host: Dr. Hans Malissa and Prof. Dr. John Lupton

Miniature solar cell (19% efficiency) which is analyzed via electrically detected magnetic resonance (EDMR). The microscopic structure of the P_b-like dangling bond defects at the (a-Si:H/c-Si) interfacs is also shown.