

Coupling of electronic and atomic degrees of freedom in quasi-1D systems from first-principles calculations

Wolf Gero Schmidt

Lehrstuhl für Theoretische Materialphysik, Universität Paderborn, 33095 Paderborn

W.G.Schmidt@upb.de

Minute structural changes may lead to drastic modifications of the electronic properties of quasi-1D systems, while, on the other hand, an electronic charge redistribution, induced, e.g. by optical excitation may induce pronounced structural modifications in such systems. This is illustrated in my talk using two prominent examples: (i) Localized photoholes at the Brillouin zone boundary of the In/Si(111)(8x2) nanowire system are shown to drive an ultrafast (8x2) $\rightarrow$ (4x1) phase transitions that is accompanied by the formation of metallic In-In bonds along the wire direction [1,2]. (ii) A $sp^3 \rightarrow sp^2+p$ rehybridization accompanied by a lateral surface charge transfer is demonstrated to destabilize the Si(553)-Au spin chains [3] with respect to a diamagnetic surface that complies with electron counting heuristics [4].

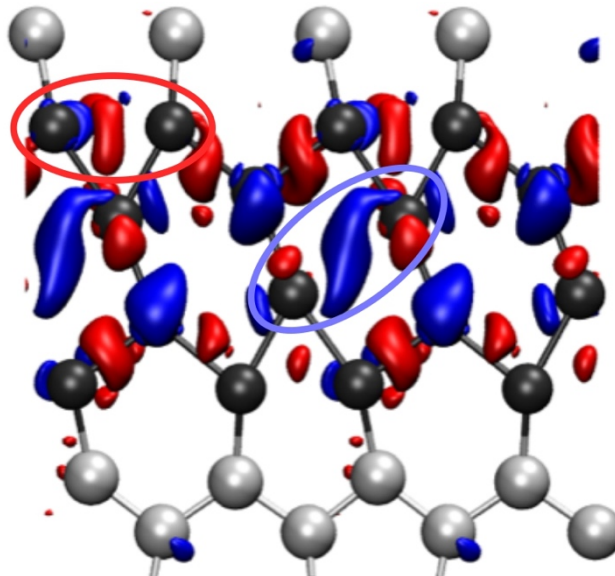


Fig. 1: Calculated charge density redistribution due to the optical excitation of the In/Si(111)(8x2) surface. Photoholes (red) reduce the strengths of outer In-In dimer bonds while charge accumulation (blue) enhances the diagonal bond across the In hexagon. This results in a (8x2) $\rightarrow$ (4x1) phase change.

- [1] T Frigge, B Hafke, T Witte, B Krenzer, C Streubühr, A Samad Syed, V Miksic Trontl, I Avigo, P Zhou, M Ligges, D von der Linde, U Bovensiepen, M Horn-von Hoegen, S Wippermann, A Lücke, S Sanna, U Gerstmann, WG Schmidt, *Nature* **544**, 207 (2017).
- [2] CW Nicholson, A Lücke, WG Schmidt, M Puppig, L Rettig, R Ernstorfer, M Wolf, *Science* **362**, 821 (2018).
- [3] SC Erwin, FJ Himpsel, *Nat. Commun.* **1**, 58 (2010).
- [4] C Braun, U Gerstmann, WG Schmidt, *Phys. Rev. B* **98**, 121402(R) (2018).