TECHNISCHE UNIVERSITÄT CHEMNITZ

PHYSIKALISCHES KOLLOQUIUM

Mittwoch, 02.05.2012, um **17:15 Uhr**

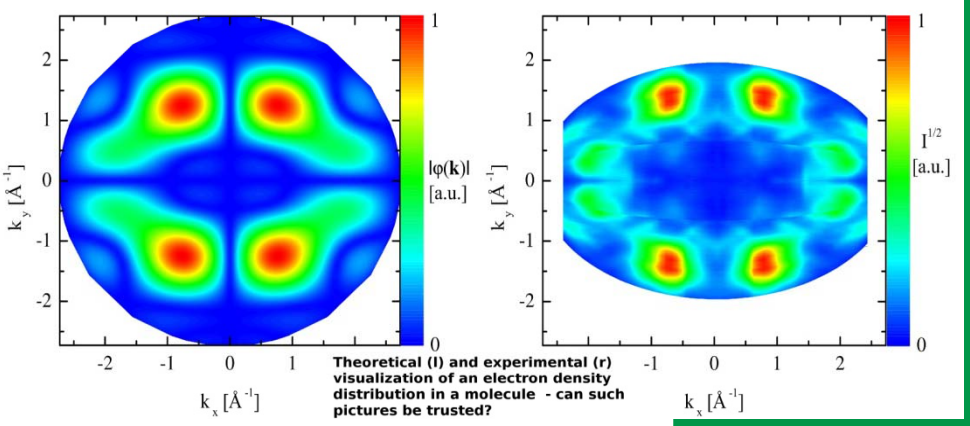
Ort: Reichenhainer Str. 90; Neues Hörsaalgebäude, Raum: 2/N013

Prof. Dr. Stephan Kümmel

Universität Bayreuth

From the laws of quantum mechanics to material properties – can theoretical physics ever bridge the gap?

The properties of new materials that exploit the special properties that matter exhibits on the nano scale offer great technological chances. Improved solar cells based on organic semiconductors or "green chemistry" based on efficient nano-particle catalysts are two prominent examples. Understanding such systems should be easy in principle, as one would "only" have to follow the rules of quantum mechanics and solve the many-particle Schrödinger equation. In practice, this is hardly possible as we are over-whelmed by the computational effort of calculating the wavefunction. Here I will argue that we can nevertheless understand nano-scale materials. On a first-principles basis by sidestepping the wavefunc-tion, and that theory allows for gaining fascinating insight into the structural and elec-tronic properties, for example of molecular semiconductors and metal clusters.



Theoretical (l) and experimental (r) visualization of an electron density distribution in a molecule - can such pictures be trusted?

Alle Zuhörer sind ab 17:00 Uhr zum Kaffee vor dem Hörsaal eingeladen.

Informationen zum Vortrag erteilt Prof. Dr. Peter Häussler, Tel.: 0371 531 33140