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Pascal Boulet

Aix-Marseille University, France

Charge density distribution as a tool for understanding relationships between structure and properties of thermoelectrics

For three decades density-functional theory (DFT) has imposed itself as an accurate quantum method to investigate materials properties from the perspective of the charge density, which is readily accessible from fast calculations. In parallel, developments of density-based descriptors such as Bader's quantum theory of atoms in molecules (QTAIM) brought new insights into materials properties. The thermoelectric properties (TE) can be evaluated from combined DFT electronic band structures calculations and Boltzmann's semi-classical formalism. It is well known that TE properties may be significantly affected by structure modifications such as doping, nano-structuring or strains application. In this lecture author will present results of TE properties calculations performed on modified materials and their relationships with the perturbations induced by these modifications on the electronic band structure and on the crystal atomic structure and bonding network investigated using Bader's theory of atoms in molecules.

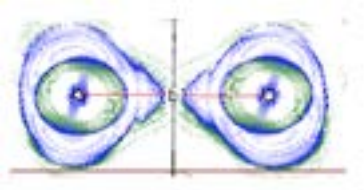

Figure: Electron density laplacian between two atoms in resonant interaction.

Recent Publications

1. Koga T, Sun X, Cronin S B and Dresselhauss M S (1999) Carrier pocket engineering applied to "strained" Si/Ge superlattices to design useful thermoelectric materials. Applied Physics Letters 75:2438-2440.
2. Heremans J P, Wiendlocha B and Chamoire A M (2012) Resonant levels in bulk thermoelectric semiconductors. Energy & Environmental Science 5:5510-5530.
3. Li H Z, Li R P, Liu J H and Huang M J (2015) Convergence of valence bands for high thermoelectric performance for p-type InN. Physica B 479:1-5.
4. Christensen M, Abrahamsen A B, Christensen N B, Juranyi F, Andersen N H, Lefmann K, Andreasson J, Bahl C R H and Iversen B B (2008) Avoided crossing of rattler modes in thermoelectric materials. Nature Materials 7:811-815

Biography

Pascal Boulet has earned his PhD thesis Diploma from both the University of Lyon, France and the University of Geneva, Switzerland in 2001 under the supervision of Prof H Chermette and Prof J Weber. His PhD thesis was related to the density-functional theory calculations on heterogeneous catalytic processes, photochemical processes in organic and organometallic species using time-dependent DFT and electron density based chemical reactivity indexes. He then moved to University College London, UK in Prof P V Coveney's group where he worked as a Postdoctoral Research Fellow on clay polymers nanocomposite materials using monte carlo and molecular dynamics simulations. From 2004 to 2017, he was Associate Professor at the University of Aix-Marseille, France where he got a full professorship position in 2017. His field of interest mainly deals with transport properties in bulk and low-dimensional materials for energy applications (thermoelectricity and photovoltaics). He has published over 60 papers in renowned journals.

pascal.boulet@univ-amu.fr

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