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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 investiga materials properties from the perspective of the charge density, which is readily accessible from fast calculations. parallel, developments of density-based descriptors such as Bader's quantum theory of atoms in molecules (QTAI brought new insights into materials properties. e 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 ma be signi cantly a ected by structure modi cations such as doping, nano-structuring or strains application. In this lecture author will present results of TE properties calculations performed on modi ed materials and their relationships with the perturbations induced by these modi cations 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/G 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 semiconductor 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 performanc 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, Ba C R H and Iversen B B (2008) Avoided crossing of rattler modes in thermoelectric materials. Nature Material 7:811-815

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