Ab-initio Modeling of Electronic Transport Properties: a Structural Informer

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Functional materials often need to be structurally adjusted for optimizing their relevant properties. In the case of a thermoelectric (TE) material, the original atomic composition and structure is modified to enhance its figure of merit $Z \cdot T = T \cdot (S^2\sigma/\kappa)$, where the Seebeck coefficient S, the electrical and thermal conductivity σ and κ are the material's transport properties. Doping is a common line of attack to optimize a TE material, and the relationship between the possible structural outcomes and the related transport properties, upon doping, may serve as a guidance to rationalize this empirical $Z \cdot T$ improvement procedure.

Recently [1] it has been shown that the *ab-initio* calculated electronic transport (ET) properties are useful *structural informers* for the doped semiconductor crystalline systems since these properties are rather sensitive to the location, the chemical nature and the concentration of the dopant atom. This fact establishes the *ab-initio* modeling as a particularly suited approach to assist the TE materials optimization.

The case of X-doped (X=Te, Sn, Fe, alkaline earth metal) $CoSb_3$ is as an interesting example of the ability of this approach to enlighten the effects the structural modifications have on a potentially highly performing TE material, especially when experiments are unable to recover detailed information on the geometric and electronic structure.

[1] Bertini L., Gatti C., *J. Chem. Phys.*, 2004, **121**, 8983.

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