Solid-state thermoelectric power generation is increasingly being seen as having potential in efficient waste-heat recovery and with that to provide alternative and cleaner forms of energy [1]. Bi$_2$Te$_3$/Sb$_2$Te$_3$ and Si/Ge heterostructures show a remarkable enhancement of the thermoelectric efficiency compared to the bulk materials [2]. While gaining much attention in the last decade, the physical origin of this enhancement is still under debate. To contribute on this, we studied the electronic structure of these heterostructures with a fully relativistic screened Korringa-Kohn-Rostoker Green’s function method. The temperature-dependent thermoelectric transport properties were calculated within the relaxation time approximation of the Boltzmann theory. The ab initio calculations were done for various superlattice periods, while the influence of interfacial strain and doping on the anisotropic thermoelectric properties was studied in detail for both material systems [3,4,5]. With Bi$_2$Te$_3$ and Sb$_2$Te$_3$ being members of the class of topological insulators [6], some insight on the thermoelectric transport of the topologically projected surface states will be given additionally.


Host: Prof. Dr. Gian Aurelio Cuniberti
Chair of Materials Science and Nanotechnology
Institute for Materials Science, TU Dresden

Contact: Dr. Dmitry Ryndyk: dmitry.ryndyk@nano.tu-dresden.de.

Everybody is very welcome!