Electricity remote from the power grid – how can computer-aided materials design help out?

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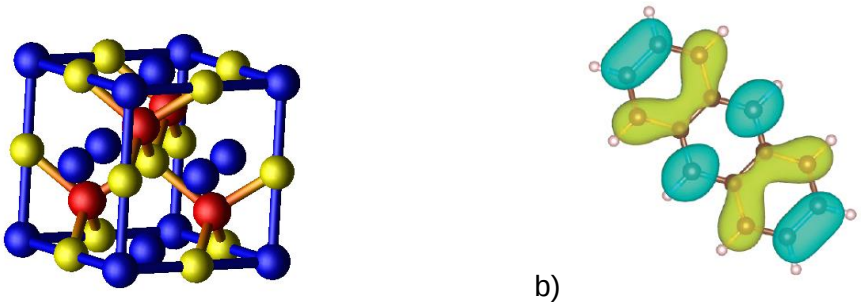
While wind farms and silicon-based photovoltaics have matured in the last decades and became the cornerstones of primary renewable energies, supplying renewable electricity to special applications, i.e. providing portable power sources for outdoor or countryside usage, still poses a challenge to materials developers.

For small amounts of electricity needed in remote places far from the power grid, converting waste heat into electricity by means of thermoelectric generators can be a robust and cost-effective solution. In my talk, I will discuss the decisive physical properties a thermoelectric material must have, and their relation to band structure. Moreover, I will present first-principles calculations with the goal to select the most suitable chemical compound from a novel class of semiconductors, ternary intermetallic compounds of a group IVb-element (Ti, Zr, Hf) with Co or Ni and Sb or Sn on inequivalent lattice sites (Fig. 1a). In the 'half-Heusler' crystal structure, these compounds develop an electronic band gap that we compute with high-level predictive tools (GW approach). Using this method [1], we predict ZrCoSb and HfNiSn to give the best performance in the p-type and n-type legs of thermoelectric generators, respectively.

Another branch of computer-aided materials development aims at light-absorbing organic materials intended for flexible solar cells or window coatings. In the later application, it is desirable to absorb only a small part of the solar light spectrum (preferentially in the UV). With this goal in mind, we carried out first-principles calculations of the energy level spacing and optical absorbance of aromatic carbon ring molecules (oligo-acenes) that absorb light in the near UV range. Exploiting the latest trend in semiconductor physics, the usage of atomically thin (2D) layers of materials as contacts, we suggest to deposit films of low-cost oligo-acenes (e.g. anthracene) on a conductive, but nearly transparent backplane of the 2D semiconductor MoS_2. First results for the adsorption energy and level alignment in heterostructures anthracene/MoS_2 will be presented.



a) b)

Figure 1 a) Crystal structure of half-Heusler compound b) lowest unoccupied orbital of anthracene

References

1. M. Zahedifar and P. Kratzer, *Phys. Rev. B* 2018, **97**, 035204.