Strengths and Limitations of Some Metals Sulfides as Abundant, Non-Toxic Materials for Photovoltaic and Thermoelectric devices

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Large deployment of waste heat recovery devices for low to medium temperature application require the identification and development of new non-toxic, low cost and earth abundant thermoelectric (TE) materials. To ensure their competitiveness, these materials have to show TE performances at least comparable to the ones of the current reference system, namely Sb or Se doped Bi_2Te_3. Accelerating the discovery of such new materials appears crucial for fulfilling the demand of the current energy market pull. In the first part of this talk, we will present the integrated computational and experimental approach we have used to search for new thermoelectric materials conforming to the boundary conditions of abundance and non-dangerousness. First principle calculations of thermoelectric transport coefficients and substitutional defect thermochemistry have been employed to screen materials with a high throughput. SnS and Bi_2S_3 have been identified as having favorable transport properties at reachable doping levels. Experimental results will be presented, confirming both the theoretical predictions and the TE potential of these two binary metal sulfides.

The second part of the talk will be dedicated to efficient Copper Zinc Tin Sulphide Selenide (CZTSSe) thin film photovoltaic devices that were fabricated with a new, fast, simple and environmentally friendly preparation method. Our process is based upon a versatile and instantaneous synthesis of a Cu-Zn-Sn-S colloid. Dispersing this colloid in a mixture of water (90%) and ethanol (10%), spraying it, and annealing sequentially the samples in two different atmospheres allow us to grow large grain crystalline layers. We measured cell efficiencies up to 9% under simulated AM1.5G (cell area 0.25 cm^2). To the best of our knowledge, this achievement represents the highest performances reached to date with CZTSSe deposited by spray, notwithstanding the unprecedented environmental friendliness of our process.