

第314回応用セラミックス研究所講演会

314th MSL Lecture

Date/Time: 10:30-11:30, Tuesday, March 15

Venue: 1F Meeting Room, Building R3

Speaker: Dr. Gilles Dennler

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Accelerated discovery of new thermoelectric materials by high throughput ab-initio computations and experimental validation

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Large deployment and penetration of waste heat recovery devices for low to medium temperature applications 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 systems, namely Sb or Se doped Bi₂Te₃. Accelerating the discovery of such new materials appears crucial for fulfilling the demand of the current energy market pull.

In the present study, we employ an integrated computational and experimental approach to search for new thermoelectric materials conforming to the boundary conditions of abundance and non-dangerousness. First principles calculations of thermoelectric transport coefficients and substitutional defect thermochemistry are used to screen metal sulfides with a high throughput. The case of a few different promising materials will be discussed in details, with a special focus upon a new ternary metal sulfide, entirely based upon low cost and non-toxic elements. We will show that by carrying out a systematic optimization of the experimental parameters upon the guidance of DFT calculations, we could achieve a power factor as high as 2.7 mW.m⁻¹.K⁻² at 540K. This is, to the best of our knowledge, the largest value ever reported on polycrystalline metal sulfides, competing directly with state-of-the-art Bi₂Te₃.

Dennler博士は、フランスのIMRA Europe S.A.S.においてCZTS等の太陽電池材料・セル構造の改善や熱電材料の合成・評価を行っております。本講演では、第一原理計算を取り入れて新しい熱電材料を効率的に探索し、その優れた性能を実験により実証した最近の成果についてお話しいたします。ふるってご参加ください。

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