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DLR – DAAD Fellowships

Fellowship No. 355

Research Area : Transportation

Research Topic: **Modelling of defects in Mg2 (Si,Sn) and their influence on the thermoelectric properties**

DLR Institute: Institute for Materials Research, DLR Cologne

Position: Doctoral Fellow

Openings: 1

Job Specification: **Thermoelectric generators** can convert heat directly into usable electrical energy. As they function without moving parts or working fluids thermoelectric generators require virtually no maintenance. They are therefore well-suited to increase the energy efficiency of various industrial processes or supply power in remote applications (space probes, space stations).
One material class of particular interest are the solid solutions based on Mg_2Si and Mg_2Sn. While these show promising thermoelectric properties the role and influence of intrinsic defects (vacancies, interstitials, anti-sites) and extrinsic defects (e.g. due to dopants) on the thermoelectric properties are still not fully understood and might be a lever to increase the material performance further.
The task of the PhD work would therefore be to elucidate the role of defects. In detail this will involve the calculation of formation energies for different defects in Mg2Si, Mg2Sn and the solid solutions using density functional theory (principally with the computer code VASP) and following from that the calculation of the transport properties based on the Boltzmann Transport Equations (BoltzTrap). The calculation of phase diagrams and the interaction of intrinsic and extrinsic dopants will be of further interest and will be tackled by a combined approach; CALPHAD + VASP. A strong interaction with experimentalists is required to validate the calculated results and design new experiments. This work will also involve a very strong collaboration with the group of Prof. Jund

at the Institut Charles Gerhardt in Montpellier (France) where most of the computer infrastructure is located

Required Qualification: MSc (or comparable) in physics, chemistry, material science or related
Background in theoretical physics/chemistry
Background in thermodynamics

Advantageous Skills: interest in experimental work
Experience with DFT calculations
Willingness for an extended stay in Montpellier, France.

English competence: fluent (see requirements on www.daad.de/dlr)

Earliest Start Date: 01.10.2018

Application Deadline: Until position filled

Further Information: http://www.dlr.de
http://www.dlr.de/wf/en/desktopdefault.aspx/tabid-1696/3089_read-3739/
https://www.icgm.fr/philippe-jund
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