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EINLADUNG zum IFP-SEMINAR

Thema: **Datamining High-Throughput DFT calculations in the search for new thermoelectric materials**

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Host: Silke Bühler-Paschen

Termin: **Mittwoch, 09. Mai 2012, 16:00 Uhr**

Ort: TU Wien, Institut für Festkörperphysik
Freihaus Seminarraum 138B, Turm C, 7. OG (rote Leitfarbe)
Wiedner Hauptstraße 8-10, 1040 Wien

Abstract:

Several thermoelectric properties of known compounds can be calculated using only the structure as an input.[1] This can used to discover potentially new thermoelectric materials by screening known structures.[2,3] However, there remains a large challenge in discovering unknown phases computationally. As ternary and higher compounds are considered, a combinatorial explosion of potential structures and combinations must be considered.

Employing a new developed high throughput environment [4] for theoretical calculations we show how the known binary silicides can be reproduced and rationalized using a systematic replacement technique. Using the Ca-Zn-Mg-Si-Sn system as an example we show how the calculated stabilities can be data-mined to produce a simple scheme for predicting the stabilities of unknown compounds.[5] This makes it possible to systematically investigate the vast number of possible ternary and higher compounds. It will be discussed how the correlations can be interpreted in terms of simplified models of the electronic structure, thereby leading to new insights into the chemistry of the system.

References :
[1] L. Bjerg, G. K. H. Madsen, and B. B. Iversen, Chem. Mater. 2011, 23, 390,
[2] G. K. H. Madsen, J. Am. Chem. Soc. 2006, 128, 12140.
[3] A. Bentien, S. Johnsen, G. K. H. Madsen, B. B. Iversen, and F. Steglich, Europhys. Lett. 2007, 80, 17008.
[4] I. Opahle, G. K. H. Madsen, R. Drautz, in preparation
[5] G. K. H. Madsen, I. Opahle, R. Drautz, in preparation

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