universität wien

Faculty of Physics

The

Computational Physics Group

cordially invites you to the talk by

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Computational thermodynamics: how to calculate phase diagrams without the fuss

Abstract

Temperature-pressure-composition phase diagrams describe the stability and equilibria of thermodynamically distinct phases, which is crucial in both academic and industrial materials science applications. In order to augment experimental studies, computer simulations and theoretical calculations are widely used to provide reference data and describe phase transitions. Although there exists a plethora of such methods, usually they can only be used to study a single type of phase transition in an optimal way, moreover, they need advance knowledge about the structure of the phases.

In recent years we have been working on adapting a novel computational sampling technique, called nested sampling, for studying atomistic systems. Nested sampling automatically generates all the relevant atomic configurations, unhindered by high barriers, and one of its most appealing advantages is that the global partition function can be calculated very easily, thus thermodynamic properties, such as the heat capacity or compressibility becomes accessible. Nested sampling samples the potential energy surface starting from the high energy region, hence no prior knowledge of the potentially stable structures is needed. This means that unlike other methods, nested sampling may be fully automated, allowing high-throughput calculations of novel materials.

Thursday, 01 February, 2018, 2:00 pm

Lecture room, Sensengasse 8, ground floor, 1090 Wien