Institute for Materials Science

Prof. Dr. Paul Erhart
Chalmers University of Technology, Gothenburg, Sweden

**Prospective topic:**
“Construction and applications of atomic scale models for materials”

Thursday, December 17th 2020
13:00 – 14:00

Normal: Seminar Room 115, Hallwachsstr. 3 (HAL)
Pandemic version: https://tinyurl.com/nanoSeminar-GA

Abstract:
Linear models, such as force constant (FC) and cluster expansions, play a key role in physics and materials science. In this talk, I will discuss methods for the systematic construction of such models as well as their application in various scenarios. Special emphasis will be put on the hiphive and icet software packages that we have developed over course of several years for this purpose. In this context, I will discuss the efficacy and efficiency of several state-of-the-art regression and feature selection methods, including methods routed in Bayesian statistics such as automatic relevance detection regression.
**Prof. Dr. Paul Erhart**

Chalmers University of Technology, Gothenburg, Sweden

**Since 2011:** Faculty member  
Department of Physics  
Chalmers University of Technology, Gothenburg, Sweden

**2009-2011:** Research staff member  
Condensed Matter and Materials Division  
Lawrence Livermore National Laboratory, California, USA

**2007-2009:** Post-doctoral fellow  
Chemistry, Materials, Earth and Life Sciences Division  
Lawrence Livermore National Laboratory, California, USA

**2006:** Ph.D. in Materials Science (Dr.-Ing.)  
Technische Universität Darmstadt, Germany