INTERDISCIPLINARY CENTRE FOR
ADVANCED MATERIALS SIMULATION

ICAMS Special Seminar

Wednesday, 13 November, 1:00 p.m.
Room IC 02-718

Professor Christoph Ortner

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Interatomic Potentials from Permutation-Invariant Polynomials

I will present the construction of interatomic potentials for materials and molecules based on a body-order expansion (ANOVA, HDRM, cluster expansion), each body order being represented by polynomials satisfying the rotation and permutation symmetry of the "exact" PES. These polynomials are determined in a data-driven fashion from linear fits trained with ab initio data. The two main issues I will discuss are (1) convergence "in theory" as well as on training sets; (2) regularisation and generalisation.
Joint work with Alice Allen (Cambridge), Gábor Csányi (Cambridge), Christoph Ortner (Warwick), and Cas van der Oord (Cambridge).