INTERDISCIPLINARY CENTRE FOR
ADVANCED MATERIALS SIMULATION

ICAMS special lecture

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at Sandia National Laboratories,
New Mexico

Tuesday, August 24, 1:30 p.m. ICAMS conference room
UHW 11/1107

Alchemical Paths and Derivatives from Density Functional Theory

Alchemical paths and derivatives hold great promise for the development of gradient based optimization algorithms in chemical compound space. I will discuss the foundation and the limits of various approaches based on density functional theory for the construction and evaluation of such quantities [1,2]. Thereafter, I will present results from applications that deal with controlling electronic structure properties, or ab initio binding energies.

[1] ``Molecular grand-canonical ensemble density functional theory and exploration of chemical space'', OAvL and M. E. Tuckerman, J. Chem. Phys. 125 154104 (2006)

[2] ``Accurate ab initio energy gradients in chemical compound space'', OAvL, J. Chem. Phys. 131 164102 (2009)