# ‘Static’ Mean-field Theory, ‘Dynamical’ Mean-field Theory, and ‘Static Dynamical’ Mean-field theory

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Abstract:
‘Quantum cluster’ methods, where fragments of a system are described with some reduced representation of the coupling to the wider environment, are one of the most promising approaches in order to take the accuracy of quantum chemistry to the extended systems required for predictive computational materials science. We will present a unified framework for these approaches, including the established ‘Dynamical mean-field theory’, and the more recent wavefunction-based alternative, ‘Density matrix embedding theory’. We will show that these can be considered in a similar framework, and a new approach can be formulated where we can arbitrarily interpolate between the physics of these two methods. We will describe the benefits of this ‘energy-weighted’ density matrix embedding, and how it solves many of the formal, conceptual, and numerical difficulties associated with both DMET and DMFT.

Refs: Booth, Fertitta, ArXiv:1808.09321 (2018)