



# PHYS: Division of Physical Chemistry

## 245 - Density matrix embedding theory: Accurate reaction paths and a second-quantized formulation for the local density of states

[View Session Detail](#)

Sebastian Wouters<sup>1,2</sup>, [sebastian.wouters@ugent.be](mailto:sebastian.wouters@ugent.be), Garnet Chan<sup>2</sup>

<sup>1</sup> Center for Molecular Modeling, Ghent University, Gent, Belgium; <sup>2</sup> Chemistry, Princeton University, Princeton, New Mexico, United States

Abstract: Density matrix embedding theory has become a viable approach to treat the correlation between finite fragments and their surrounding molecular or lattice environments. In this talk, both the DMET ground-state and spectral function algorithms will be discussed from a quantum chemical perspective. A formulation in terms of orbital-based second-quantized Hamiltonians, i.e. the usual one- and two-electron integrals in quantum chemistry, allows to recycle existing correlated implementations to solve the ground-state and response impurity problems to obtain spectral functions. Results for an  $S_N2$  reaction path and the local density of states for a lattice Hamiltonian will be presented.

[Home](#)

[Schedule](#)

[Floor Plans](#)

[Search](#)

[More ..](#)