

## Contribution submission to the conference Berlin 2018

**Selfconsistent density embedding - a new class of functionals for DFT** — ●ULIANA MORDOVINA<sup>1</sup>, TERESA E. REINHARD<sup>1</sup>, HEIKO APPEL<sup>1</sup>, and ANGEL RUBIO<sup>1,2</sup> — <sup>1</sup>Max Planck Institute for the Structure and Dynamics of Matter, Hamburg, Germany — <sup>2</sup>Center for Computational Quantum Physics (CCQ), The Flatiron Institute, 162 Fifth Avenue, New York NY 10010, USA — <sup>3</sup>Nano-bio Spectroscopy Group and ETSF, Departamento de Fisica de Materiales, Universidad del Pais Vasco UPV/EHU, San Sebastian, Spain

We propose a new technique to find functionals for density functional theory (DFT) in an ab-initio fashion. This technique origins in the recently developed density-matrix embedding theory (DMET) [1]. DMET is a quantum-in-quantum embedding method, which is based on finding a projection between the high-dimensional wave function of the full system and a lower-dimensional wavefunction living in the active space of the embedded system, which is then solved exactly. In the original DMET scope, the projection is improved via optimization of the reduced one-body density matrix. We replace this optimization by a density inversion, exploiting the one-to-one mapping between electronic density and Kohn-Sham potential.

The proposed density-embedding scheme serves as functional in DFT, which, unlike in usual DFT, can be systematically improved by increasing the size of the active space.

We show convergence toward exact results for 1D systems as well as results for 2D systems.

[1] G. Knizia, G. K.-L Chan, Phys. Rev. Lett 109, 186404, (2012)

**Part:** O  
**Type:** Vortrag;Talk  
**Topic:** Focus session: Frontiers of Electronic-Structure Theory: New Concepts and Developments in Density Functional Theory and Beyond  
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