Playing with the reduced density-matrix: representability, functionals and embedding

Matthieu Saubanère*1

1Institut Charles Gerhardt Montpellier - Institut de Chimie Moléculaire et des Matériaux de Montpellier – Ecole Nationale Supérieure de Chimie de Montpellier, Université de Montpellier, Centre National de la Recherche Scientifique : UMR5253 – France

Résumé

Going beyond Density-Functional Theory appear today as an important challenge for theoretical chemists and physicists, in particular to improve the accurate for strongly correlated systems and to access to beyond ground-states properties. In that context, theories based on the reduced density-matrix are appealing but necessitates developments to become practical. In this presentation we present our recent work on the resolution of the density matrix functional theory variational equations and our strategy to construct a density-matrix-based embedding theory. Proofs of concept are presented in the framework of the periodic Hubbard model.