Master 2 Internship

Title: **Interaction energy functionals from the homogeneous electron gas**

Type: **theoretical**

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PhD funding (if any): **yes**

Key word : Electronic structure theory; Density Functional Theory; Strongly interacting system; Condensed matter theory; Computational physic.

Project: Over the last two decades, density functional theory (DFT) has played a major role in the study of the physico-chemical properties of molecules and materials. The key idea behind DFT is to replace the wavefunction with the electronic density as the fundamental variable of the many-electron problem. Within the Kohn–Sham decomposition scheme, electronic repulsion effects are treated implicitly by a Hartree-exchange-correlation (Hxc) functional of the density, leading to a good balance between computational cost and accuracy. However, despite the numerous Hxc functionals developed over the past decades, KS-DFT still faces challenges when dealing with systems that exhibit strong (or static) correlation effects.

Alternatively, replacing the density with the one-particle reduced density matrix (1-RDM) as the fundamental variable leads to 1-RDM functional theory (1-RDMFT), which offers several advantages. In particular, the kinetic and exchange energy contributions are expressed exactly and analytically with respect to the 1-RDM. However, in line with the Hartree-Fock approximation, most interaction energy functionals of the 1-RDM are based on the concept of natural orbital occupations. The most recent and efficient ones are the Piris natural orbital functionals (PNOFs), which are based on cumulants. Despite promising results, natural orbital functionals (NOFs) in general do not perform well across all correlation regimes, although recent progress is worth noting.

This internship will explore the possibility of designing interaction energy functionals of the 1-RDM based on the homogeneous interacting electron gas. The strategy consists in relating numerical results obtained at the Random Phase Approximation or GW level with theoretical concepts of Nearsightedness, scaling lows and/or Virial relations.

Possibility to pursue a PhD in a related topic on the electronic structure theory of solids using quantum computers.