Title: Green's function functionals as density functionals

Name: Steven Crisostomo
Affiliation: University of California, Irvine

Using exact density functional theory, we formalize a theory of Green's function (GF) functionals. We explore self-energies along traditional lines, as functionals of bare or interacting GFs, and develop a density-functional counterpart, following our recent work [arXiv:2403.03364 (2024)]. The density functional constructions are inherently non-diagrammatic and don't require convergence of an underlying perturbation theory. Keeping careful track of GF and density functional dependence, we examine the self-energy corrections associated with the fixed-density adiabatic connection formalism. Lastly, we derive a density-functional version of the Luttinger-Ward (LW) functional, which differs considerably from the construction first proposed by Sham [*Phys. Rev. B* **32**, 3876 (1985)]. We illustrate exact results using a two-site Hubbard model.

This work is in collaboration with Kieron Burke and Hardy Gross, and is supported by NSF Award No. CHE-2154371.