

Make DFT Great Again

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In this talk, I will summarize our recent efforts to generalize the foundation and applications of density functional theory (DFT). From the perspective of quantum information theory, DFT can be regarded as a quantum tomography technique, which aims to reconstruct properties of a quantum many-body system from measurements on some local expectation values. Then, a fundamental question is whether a generalized version of DFT in principle exists for an arbitrary quantum system. Answering this question leads to an interesting “all-or-nothing” classification, as well as new density functionals and Kohn-Sham auxiliary systems, beyond the conventional electron gas setup. These explorations remind us that being the founder of DFT Walter Kohn’s real ambition is to attack the quantum many-body problem from a unique angle. Bearing this spirit, we will carry on the banner of DFT and make it great again.