Density Functional Theory: Background, Challenges, and Some Success

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This talk will introduce density functional theory, motivate our work to improve it and provide concrete examples of some of its more interesting successes and applications. In particular, it will discuss a set of new hybrid meta exchange correlation functionals that are parametrized for a whole range of systems including both transition metals and nonmetals. We will assess their performance on the basis of their ability to predict geometries, thermochemistry, kinetics, noncovalent interactions, transition metal bonding, metal atom excitation energies, and molecular excitation energies to valence and Rydberg states.