

# Recent Advances in Kohn-Sham Density Functional Theory and Multiconfiguration Pair-Density Functional Theory

Donald G. Truhlar

Department of Chemistry, Chemical Theory Center, and Supercomputing Institute,  
University of Minnesota, Minneapolis, MN 55355-0431

Kohn-Sham density functional theory has revolutionized the practice of quantum electronic structure in both chemistry and physics, and the accuracy depends on the quality of the exchange-correlation functional. I will review recent progress including the recently developed specialized functionals xe-PBE0, HLE16, and HLE17 and the recently developed “universal” functionals GAM, MN15-L, and MN15. Although the new functionals have provided significant progress in treating strongly correlated (i.e., inherently multiconfigurational) systems and excited states, these remain difficult for Kohn-Sham theory. To remedy this, we have developed a new form of density functional theory (multiconfiguration pair-density functional theory: MC-PDFT) based on multiconfiguration wave functions and the on-top pair density, and my talk will also review recent progress with this new theoretical formalism.

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