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New Density Functionals with Broad Applicability in Chemistry (SOGGA11, SOGGA11-X, M11, M11-L) and Approaches to Open-Shell DFT[1]

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The accuracy of density functional theory for practical applications is determined by the quality of the necessarily approximate exchange-correlation functional ("density functional") being used, and the goal of functional development in chemical physics is to obtain a functional that is accurate for a broad range of chemistry and physics. In our work we consider molecular structures and solid-state lattice constants and band gaps, but we emphasize energetics for main-group and transition-metal chemistry, including thermochemistry and barrier heights, noncovalent interaction energies, and excitation energies. This lecture will discuss four new density functionals, each optimized to give the best across-the-board performance for a broad range of chemistry in their class of functional: SOGGA11, a generalized gradient approximation (GGA); SOGGA11-X, a global hybrid GGA; M11: a range-separated hybrid meta-GGA, and M11-L, a meta-GGA. SOGGA11 and M11-L are local functionals, and SOGGA11-X and M11 include some nonlocal Hartree–Fock exchange. To the extent that time permits, I may also discuss recent progress in the treatment of open-shell systems by density functional theory, including time-dependent DFT, open-shell SCF, and noncollinear DFT. This invited lecture is based on collaborative research carried out with Roberto Peverati, Sijie Luo, Ke Yang, Boris Averkiev, Yan Zhao, and Rosendo Valero.

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