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Recent progress in density functional theory[1]

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Ongoing work involves several areas of density functional theory: new methods for computing electronic excitation energies, including a new way to remove spin contamination in the spin-flip Tamm-Dancoff approximation and a configuration-interaction-corrected Tamm-Dancoff Approximation for treating conical intersections; new ways to treat open-shell states, including a reinterpreted broken-symmetry method and multi-configuration Kohn-Sham theory; a new exchange-correlation functional; new tests of density functional theory against databases for electronic transition energies and molecules and solids containing metal atoms; and applications. A selection of results will be presented. I am grateful to the following collaborators for contributions to the ongoing work: Boris Averkiev, Rebecca Carlson, Laura Fernandez, Laura Gagliardi, Chad Hoyer, Francesc Illas, Miho Isegawa, Shaohong Li, Giovanni Li Manni, Sijie Luo, Dongxia Ma, Remi Maurice, Rubén Means-Pañeda, Roberto Peverati, Nora Planas, Prasenjit Seal, Pragya Verma, Bo Wang, Xuefei Xu, Ke R. Yang, Haoyu Yu, Wenjing Zhang, and Jingjing Zheng.

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