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DFT methods for conjugated materials: From benchmarks to functionals JOHN SEARS, School of Chemistry and Biochemistry, Georgia Institute of Technology, Atlanta, Georgia 30332-0400, JEAN-LUC BREDAS, School of Chemistry and Biochemistry, Georgia Institute of Technology — From a theoretical standpoint, many of the problems of interest in the study of pi-conjugated materials for organic electronics applications pose a particular challenge for many modern density functional theory methods. Systematic errors have been observed, for instance, in the description of charge-transfer excitations at donor/acceptor interfaces, in linear and non-linear polarizabilites, as well as in the geometric and electronic properties of conjugated polymers [1,2]. We will discuss recent results in our lab aimed at: (i) understanding the sources of error for some of these problems; (ii) addressing these errors using tuned long-range corrected functionals; and (iii) using these results to guide the development of state-of-the-art methodologies in a new open-source DFT code.

[1] J. S. Sears, T. Korzdorfer, C. R. Zhang, and J. L. Bredas, J. Chem. Phys. 135 151103 (2011)
[2] T. Korzdorfer, J. S. Sears, C. Sutton, and J. L. Bredas, J. Chem. Phys., accepted.

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