Abstract Submitted
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Benchmarks and applications of novel density functionals to semiconducting polymers[1] BENJAMIN JANESKO, Texas Christian University — Semiconducting polymers show substantial promise as the active ingredients in inexpensive, flexible, processable "plastic electronics" and "plastic solar cells." The difficulty and expense of polymer synthesis makes computational prescreening of novel polymer candidates essential for guiding experiment. Density functional theory (DFT), particularly using hybrid exchange-correlation functionals, has been broadly applied to modeling isolated polymer chains. However, these functionals can be formally and computationally problematic for bulk polymers associating via noncovalent interactions. Screened hybrid and "Rung 3.5" density functionals, particularly their dispersion-corrected variants, show promise for ameliorating these limitations. This work presents benchmarks of these new functionals for this problem, and applications to novel conjugated and nonconjugated semiconducting polymers.

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