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**Performance of optimally-tuned range-separated hybrid functionals in predicting molecular valence-electron spectra** DAVID A. EGGER, Weizmann Institute of Science, Israel and Graz University of Technology, Austria, SHIRA WEISSMAN, SIVAN REFAELY-ABRAMSON, Weizmann Institute of Science, Israel, SAHAR SHARIFZADEH, Molecular Foundry, Lawrence Berkeley National Laboratory, MATTHIAS DAUTH, University of Bayreuth, Germany, ROI BAER, Hebrew University of Jerusalem, Israel, STEPHAN KUEMMEL, University of Bayreuth, Germany, JEFFREY B. NEATON, Molecular Foundry, Lawrence Berkeley National Laboratory, EGBERT ZOJER, Graz University of Technology, Austria, LEEOR KRONIK, Weizmann Institute of Science, Israel — Density functional theory with optimally-tuned range-separated hybrid (OT-RSH) functionals has been recently suggested [Phys. Rev. Lett. 109, 226405 (2012)] as a non-empirical approach to accurately predict the outer-valence electronic structure of molecules. Here, we provide a quantitative evaluation of the OT-RSH approach by examining its performance in predicting the outer-valence electron spectra of prototypical gas-phase aromatic rings. For a range of up to several eV, we find that the obtained outer-valence electronic structure agrees very well (typically within 0.1-0.2 eV) with both experimental photoemission and theoretical GW data. The sole exception found is a high-symmetry orbital that is particular to aromatic rings and occurs relatively deep inside the valence state manifold. We conclude that OT-RSH functionals offer a balanced description of differently localized electronic states, a feature we find to prevail also for the more complex terpyrimidinethiol.

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