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Electronic structure of CuPc from an optimally-tuned range-separated hybrid functional SHIRA WEISSMAN, SIVAN REFAELY-ABRAMSON, Department of Materials and Interfaces, Weizmann Institute of Science, Rehovoth 76100, Israel, DAVID A. EGGER[1], EGBERT ZOJER, Institute of Solid State Physics, Graz University of Technology, 8010 Graz, Austria, LEEOR KRONIK, Department of Materials and Interfaces, Weizmann Institute of Science, Rehovoth 76100, Israel — The optimally-tuned range separated hybrid (RSH) functional approach [1] was recently shown to allow for the calculation of the outer valence electronic spectrum of different molecules [2], resulting in good agreement with both experiment and many-body perturbation theory. The functional is based on a separation of short-range and long-range exchange components, where the range-separation parameters is tuned based on satisfaction of physical constraints, notably the ionization potential theorem. Here, we apply this approach to copper phthalocyanine (CuPc), which is of much recent interest owing to its ability to form a highly stable organic semiconductor. CuPc offers a difficult challenge for the method, because it is an open shell molecule whose electronic structure involves strongly localized d orbitals. We find that the spectrum obtained for CuPc using the optimally-tuned RSH functional is in very good agreement with both experiment and MBPT calculations throughout most of the outer valence range. [1] L.Kronik, T.Stein, S.Refaely-Abramson, R.Baer,*J. Chem. Theo. Comp.* (Perspectives Article) **8**, 1515 (2012). [2] S.Refaely-Abramson, S.Sharifzadeh, N.Govind, J.Autschbach, J.B.Neaton, R.Baer, L.Kronik, *Phys. Rev. Lett.* **109**, 226405 (2012)

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