

Abstract Submitted  
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**Spectroscopic Fingerprinting of Small Molecules via Many-Body Perturbation Theory** PETER DOAK, Molecular Foundry, LBNL; Department of Chemistry, UC-Berkeley, PIERRE DARANCET, JEFFREY NEATON, Molecular Foundry, LBNL — Quantitative understanding of the photophysics of small organic molecules is an important challenge and relevant to a range of energy conversion applications. Existing first-principles methods, such as time-dependent density functional theory, coupled cluster, and other quantum chemistry-based approaches can sometimes provide onset energies with good accuracy, but agreement at higher energies - a more complete spectral fingerprint - is frequently less adequate. Here we use DFT and many-body perturbation theory, within the GW approximation and the Bethe-Salpeter Equation approach, to compute the UV-Vis absorption spectra for a range of small molecules, comparing closely to room-temperature, solution-phase measurements of onsets and spectra. First-principles molecular dynamics is used to prepare snapshots of finite temperature conformations. The effects of continuum and explicit solvation models are considered. The importance of dynamic disorder, delocalized unoccupied states, and solvation are thoroughly discussed in the context of experiments. Support: DOE via the Molecular Foundry and Helios SERC, and NSF via NCN. Computational support provided by NERSC.

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