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**Photo-induced Charge Separation in Nanoscale Donor-Bridge-Acceptor Systems: Theory and Experiment** PETER DOAK, Molecular Foundry, LBNL; Department of Chemistry, UC-Berkeley, PIERRE DARANCET, Molecular Foundry, LBNL, KASPER MOTH-POULSEN, Department of Chemical and Biological Engineering, Chalmers U. of Technology, JESSE JENKINS, Department of Chemistry, UC-Berkeley, RACHEL SEGALMAN, Department of Chemical Engineering, UC-Berkeley, DON TILLEY, Department of Chemistry, UC-Berkeley, JEFF NEATON, Molecular Foundry, LBNL — Understanding and control of light-harvesting processes at the molecular-scale remains a fundamental challenge in solar energy conversion. Donor-bridge-acceptor molecules (DBAM), with atomically-defined interfaces made by a covalently bound bridge between donor and acceptor moieties, allow probing of excited states relevant to optical absorption and charge separation. In close collaboration with experiment, we use first-principles many-body perturbation theory, within the GW approximation and the Bethe-Salpeter equation approach, to compute excited states for six DBAMs. We compare with experiments, and quantitative agreement is obtained. Implications of our results for nanoscale light-harvesting are thoroughly discussed. Support: DOE via the Molecular Foundry and Helios SERC, and NSF via NCN. Computational support provided by NERSC.

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