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The influence of excitonic effects on charge separation at hybrid nanoscale interfaces[1] ZHIGANG WU, HUASHAN LI, MARK LUSK, Colorado School of Mines — Efficient charge separation is critical in nanostructured photovoltaic systems, but the accurate prediction of charge separation rates remains an extremely difficult task. Although considerable progress has been made, reliable theoretical schemes to describe the charge-separation mechanisms and to compute the interfacial charge transfer dynamics have not been fully developed. In this work, we embrace the excitonic effects that are of critical importance in nanoscale geometries to derive a criterion for charge separation at hybrid nanoscale interfaces beyond the traditional quasiparticle energy-level alignment. The approach utilizes calculations from many-body perturbation theory with Green functions to accurately account for self-energy and electron-hole interactions. Four representative interfaces between Si quantum dots and small molecules are considered using this approach, in order to demonstrate that both excitonic and Coulomb stabilization effects are essential for correctly predicting charge separation at nanostructured interfaces. Interestingly, our calculations suggest that preemptory exciton transfer across interfaces only suppresses the subsequent charge separation. We also compute charge separation rates using the Marcus theory and other methods, and their accuracy an

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