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Designing TMDC-organic interfaces for effective charge transfer.[1] KUSHAL RIJAL, FATIMAH RUDAYNI, TIKA RAM KAFLE, WAI-LUN CHAN, University of Kansas — Excited-state electron transfer (ET) across molecules/transition metal dichalcogenide crystal (TMDC) interfaces is a critical process for the functioning of various organic/TMDC hybrid optoelectronic devices. Therefore, it is important to understand the fundamental factors that can facilitate or limit the ET rate. Here it is found that an undesirable combination of the interfacial band offset and the spatial dimensionality of the delocalized electron wave function can significantly slow down the ET process. Specifically, it is found that whereas the ET rate from TMDCs (MoS2 and WSe2) to fullerenes is relative insensitive to the band offset, the ET rate from TMDCs to perylene molecules can be reduced by an order of magnitude when the band offset is large. For the perylene crystal, the sensitivity of the ET rate on the band offset is explained by the 1D nature of the electronic wave function, which limits the availability of states with the appropriate energy to accept the electron.

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