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Ab-initio modelling of solvent effects in pentacene-derived systems in the context of singlet fission[1] DAVID H P TURBAN, Univ of Cambridge, NICHOLAS D M HINE, Univ of Warwick — Singlet fission (SF) is a multiexciton generation process that could be harnessed to improve the efficiency of photovoltaic devices. Experimentally, systems derived from the pentacene molecule have been shown to exhibit ultrafast SF with high yields. It has become apparent that the excited states and thereby SF is strongly affected by the molecular environment. This means that modelling approaches that restrict attention to only a few molecules for tractability are severely limited. In order to overcome this limitation we harness excited-state linear-scaling DFT (as implemented in the ONETEP code), combined with empirical MD to sample configurations of the environment. Specifically, we use constrained DFT and time-dependent DFT to model the excited electronic states relevant for SF. We investigate how these states are affected by the explicitly modelled molecular environment and the implications for fission.

[1]Engineering and Physical Sciences Research Council, Winton Programme for the Physics of Sustainability

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