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Explicit crystal host effects on excited state properties of linear polyacenes: towards a room-temperature maser ROBERT CHARLTON, STUART BOGATKO, Imperial College London, TIM ZUEHLSDORFF, University of California, Merced, NICHOLAS HINE, University of Warwick, ANDREW HORSFIELD, PETER HAYNES, Imperial College London — Maser technology has been held back for decades by the impracticality of the operating conditions of traditional masing devices, such as cryogenic freezing and strong magnetic fields. Recently it has been experimentally demonstrated that pentacene in *p*-terphenyl can act as a viable solid-state room-temperature maser by exploiting the alignment of the low-lying singlet and triplet excited states of pentacene. To understand the operation of this device from first principles, an *ab initio* study of the excitonic properties of pentacene in *p*-terphenyl has been carried out using time-dependent density functional theory (TDDFT), implemented in the linear-scaling ONETEP software (www.onetep.org). In particular, we focus on the impact that the wider crystal has on the localised pentacene excitations by performing an explicit DFT treatment of the *p*-terphenyl environment. We demonstrate the importance of explicit crystal host effects in calculating the excitation energies of pentacene in *p*-terphenyl, providing important information for the operation of the maser. We then use this same approach to test the viability of other linear polyacenes as maser candidates as a screening step before experimental testing.

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