Organic Solar Cells Based on π-Conjugated Semiconductors: The Binary PM6:Y6 Mixture as a Case Study

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The urgent need for an energetical transition has propelled our modern world, dependent on fossil fuels, into a new era that gives room for renewable energies. Among them, solar energy is the most reliable energy resource. Organic donor and acceptor molecules are promising materials for low-cost and scalable organic solar cells (OSCs), which are vital for the development of safe and efficient power generation infrastructures of the future. Yet the power conversion efficiency (PCE) of first-generation fullerene-based OSCs is severely undermined by structural degradation and poor morphology control at the molecular level, hence barely reaching 12%.

In the last decades, immense effort and creativity have been deployed to prepare OSCs with improved PCEs, namely by mixing different non-fullerene acceptors (NFAs) and polymer donors in binary and ternary blends. A large number of acceptor-donor mixtures have been proposed and investigated. Herein, we use molecular dynamics simulation to study the PM6:Y6 binary mixture. We review the computational works that have been reported to date and discuss the structural and electronic effects of the pi-conjugation in these compounds, a prominent feature that promotes their solid-state arrangement into crystalline films, favoring the stability and good performance of the mixture. The comprehensive fundamental understanding of this system guides the next steps toward the design of new-generation OSCs.