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Further Study of Mechanism of Contrasting Charge Transport Properties for Phenyl and Thienyl Substituent Organic Semiconductors

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Abstract : Based on the previous work about the influence mechanism of the mobility difference of phenyl and thienyl substituent semiconductors, we have made further exploration towards to design high-performance organic thin-film transistors. The substituent groups effect plays a significant role in materials properties and device performance as well. For the theoretical study, simulation of materials property and crystal packing can supply scientific guidance for materials synthesis in experiments. This time, we have taken the computational methods to design a new material substituent with furan groups, which are the potential to be used in organic thin-film transistors and organic single-crystal transistors. The reorganization energy has been calculated and much lower than 2,6-diphenyl anthracene (DPAnt), which performs large mobility as more than 30 $cm^2V^{-1}s^{-1}$. Moreover, the other important parameter, charge transfer integral is larger than DPAnt, which suggested the furan substituent material may get a much better charge transport data. On the whole, the mechanism investigation based on phenyl and thienyl assisted in designing novel materials with furan substituent, which is predicted to be an outperformed organic field-effect transistors.

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