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Theoretical Prediction of Crystal Structures of Semiconducting Aromatic Compounds

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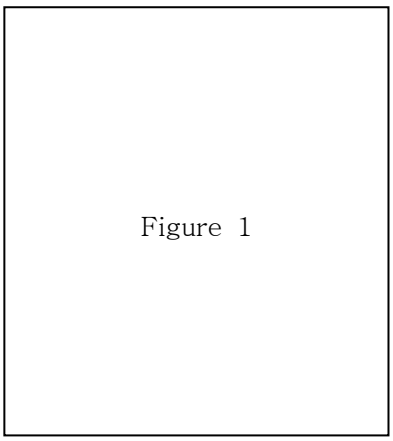

The molecular arrangement is one of the key factors controlling various properties in organic materials. Therefore, the theoretical prediction of crystal structures and molecular arrangements has a potential to become a useful tool for designing organic materials, although it is still challenging. In this work, we theoretically predict the crystal structures of semiconducting aromatic compounds and compare their molecular arrangements with experimentally determined ones [1]. We demonstrated that this method successfully determines the crystal structures of pentacene and rubrene: In each compound, the predicted crystal structure with the most stable potential energy is in good agreement with experimental structure. In rubrene, the tetracene backbone takes fairly flat conformation in crystal due to intermolecular interactions, in contrast to more twisted conformation in gas phase. This significant conformational change is well predicted in the calculation. We will extend our investigation to other semiconducting aromatic compounds.

[1] S. Obata, T. Miura, Y. Shimoi, *Jpn. J. Appl. Phys.* **53** 01AD02 (2014).

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