Theoretical Evaluation of the Relationships between Structure and Charge Transport Properties in Organic Devices

Sang Uck Lee[1,2*]
[1]Department of Bionano Technology, Hanyang, Ansan 426791
[2] Department of Chemical and Molecular Engineering, Hanyang University, Ansan 426791
Phone +82 31 400 5501, [*]E-Mail: sulee@hanyang.ac.kr

Abstract

Electronic devices based on organic semiconductors have been actively explored for flexible, transparent and low-cost electronic applications. However to realize such applications, the charge transport properties of organic semiconductors must be improved. At the microscopic level, one of the major factors governing the charge transport properties is the amplitude of the electronic transfer integral *t*, which expresses the ease of transfer of a charge between two interacting molecules. Consequently, the charge transport properties of organic semiconductors critically depend on their molecular packing structures, such as π-π stacking distance and π-π overlap degree. Therefore, tremendous progress toward high-performance organic electronics has been achieved by increasing the charge transport properties through rational design of organic molecules and morphology control of organic crystals. In addition, much attention has been drawn to study charge transport in organic semiconductors in order to find fundamental routes to develop high-performance organic electronics based on an understanding of the intermolecular interactions and the structure-property relationships.

Here I demonstrate new approach for controlling organic crystal morphology using eutectic crystallization and provide fundamental understanding of the structure-charge transport property relationships in organic crystals.

Keywords: Density functional theory, charge transport, organic electronics, organic crystal.