

Theory of charge transport in carbon electronic materials

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Abstrak

This volume describes recent progresses in Prof. Shuai's group in developing computational tools to assess the intrinsic carrier mobility for organic and carbon materials at the first-principles level. According to the electron-phonon coupling strength, the charge transport mechanism is classified into three different categories, namely, the localized hopping model, the extended band model, and the polaron model. For each of them, a corresponding theoretical approach is developed and implemented into typical examples.