

Preface

Organic electronics has been extensively studied for over 50 years, and is now still a rapidly developing area. Charge carrier mobility is at the center of these electronic devices. This book describes recent progresses 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, we classify the charge transport mechanism into three different categories, namely, the localized hopping model, the extended band model, and the polaron model. For each of them, we develop a corresponding theoretical approach and implement it to typical examples. A lot of successes have been achieved and the outlook is given. The authors are deeply grateful to the following collaborators: Dr. Mengqiu Long and Dr. Ling Tang, postdoctoral fellows in Shuai’s group, working on developing deformation potential theory applied to organic and carbon materials; Dr. Shiwei Yin, Dr. Guangjun Nan and Dr. Xiaodi Yang, former PhD students in Shuai’s group, working on developing intermolecular coupling quantum chemistry method, random walk simulation, and quantum nuclear tunneling effects within hopping scheme, respectively. The financial supports come from the National Natural Science Foundation of China, the Ministry of Science and Technology of China, the Chinese Academy of Sciences, the European Union sixth Framework, and Solvay. We are glad to receive any helpful suggestions and comments from the readers.

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