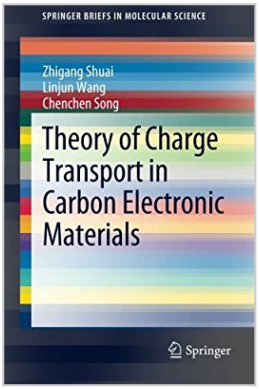

Theory of Charge Transport in Carbon Electronic Materials (SpringerBriefs in Molecular Science)

By Zhigang Shuai, Linjun Wang, Chenchen Song

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Mechanism of charge transport in organic solids has been an issue of intensive interests and debates for over 50 years, not only because of the applications in printing electronics, but also because of the great challenges in understanding the electronic processes in complex systems. With the fast developments of both electronic structure theory and the computational technology, the dream of predicting the charge mobility is now gradually becoming a reality. 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.

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Editorial Review

From the Back Cover

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About the Author

Prof. Zhigang Shuai received his PhD from Fudan University in 1989. From 1990 to 2001, he worked at the Laboratory of Chemistry for Novel Materials, University of Mons, Belgium, as a postdoc and then as a senior research associate with Prof. Jean-Luc Brédas. Since 2002, he became a full professor at the Institute of Chemistry of the Chinese Academy of Sciences (CAS) in Beijing, under the support of “Hundred Talent Program”. Since May 2008, he became a full professor (Changjiang Scholar) at the Department of Chemistry, Tsinghua University.
Prof. Shuai is an elected member of the International Academy of Quantum Molecular Science (2008) and a fellow of the Royal Society of Chemistry (2009).
Prof. Shuai is the Associate Editor-in-Chief of Frontiers of Chemistry in China, and member of editorial boards of the following scientific journals: Theoretical Chemistry Accounts, Journal of Theoretical and Computational Chemistry, Science in China-Chemistry, Progress of Chemistry, Acta Phys.-Chim. Sinica, Journal of Molecular Science.
Prof. Shuai's research interests are theoretical chemistry and modeling of the organic and polymeric functional materials. He has published more than 230 papers with more than 4900 citations (H-factor=36), and delivered invited lectures at more than 30 international conferences.

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