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"Quantitative computation of light-emitting efficiency and carrier mobility for organic materials"

We present our recent work on the computational investigations on the light-emitting efficiency and charge carrier mobility for organic optoelectronic materials. We developed a time-dependent vibration correlation function formalism for evaluating the molecular excited state non-radiative decay rate combining non-adiabatic coupling and spin-orbit coupling, to make quantitative prediction for light-emitting quantum efficiency. We further improved the computational methods by going beyond the localized semiclassical Marcus limit to describe the charge transport in organic semiconductors.

Biosketch

Zhigang Shuai is a Changjiang Scholar Chair Professor in the Department of Chemistry, Tsinghua University in Beijing. His research interests focus on the development of computational methodologies for modeling functional materials. He has devised computational schemes for the luminescence spectra and quantum efficiency, carrier mobility, thermoelectric conversion, and photovoltaic processes in organic/polymeric materials. He extended the density matrix renormalization group theory for the excited state structures for conjugated polymers. He has published more than 340 articles with an H-index 64.

He was elected to the International Academy of Quantum Molecular Science (2008), Fellow of the Royal Society of Chemistry (2009), Foreign Member of the Academia Europaea (2011), the Royal Academy of Belgium (2013), and the Scientific Board of WATOC (2017). He was the recipient of the National Outstanding Young Scientist Fund (2004), National Talent Program of the Ministry of Personnel (2006), and the Chinese Chemical Society – AkzoNobel Chemical Sciences Award (2012). He is the Associate Editor of the Journal of Materials Chemistry A and Acta Chimica Sinica. He serves as editorial/advisory board member for the following scientific journals: National Science Review, J Phys Chem, Chem Phys Lett, Theor Chem Acc, WIRES Comput Mol Sci, Advanced Theory and Simulation, Nanoscale, J Mater Chem C, Chem Asian J, China Science Bulletin.

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