Modeling organic functional materials: light-emitting efficiency and carrier transport

Zhigang Shuai*†[1]

[1]Tsinghua University (Tsinghua) – Department of Chemistry, Tsinghua University, 100084 Beijing, Chine

Résumé

Electronic non-adiabatic processes govern the optoelectronic properties for organic semiconductors, such as carrier transport and light emitting. I will describe three methodologies we developed recently for computational assessments of (i) charge transport mobility of organic materials in the hopping limit where we highlight the nuclear tunneling effect and we predict the isotope effect [1]; (ii) charge and heat transport in organic/carbon materials in the bandlike limit for predictions of mobility and thermoelectric figure of merits [2]; (iii) and the radiative and non-radiative decay rates for both fluorescence and phosphorescence under the distorted and displaced harmonic model. Quantitative prediction of luminescence efficiency is made possible through first-principles calculation and the aggregation-induced emission phenomenon is accounted quantitatively [3].

References

Z Shuai, et al., "From charge transport parameters to charge mobility in organic semconductors through multiscale simulation", Chem Soc Rev 2014, 43, 2662-2679.

Z. Shuai, et al.; Acc. Chem Res. 2014, doi:10.1021/ar400306k.

Z. Shuai and Q. Peng, Physics Reports, 2014, 537, 123-156

Mots-Clés: organic functional materials, light, emitting efficiency, carrier transport

*Intervenant

†Auteur correspondant: zgshuai@tsinghua.edu.cn