Multireference Methods in Organic Electronics and Photonics

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The computational problems that typically arise in organic electronics are the problems of light absorption and emission, charge separation and recombination, and charge transport. These problems are usually addressed with the relatively cheap and fast density functional theory, which allows for large-scale calculations. However, this approach has intrinsic deficiencies that lead to qualitatively wrong results. Among these are overestimation of charge delocalization in extended molecular systems, underestimation of the energy of charge-transfer states, and different errors in the energies of singlet and triplet states, which lead to wrong transition probabilities of nonradiative processes.

Multireference methods, such as CASSCF/XMCQDPT, provide qualitatively correct and accurate description of the processes of interest. In particular, they correctly describe charge and exciton localization in extended systems through including the states with different localization with equal weights. They also provide balanced treatment of states of different multiplicity and different orbital character. Therefore, multireference methods give deeper insight into the nature of the systems under study. Understanding the mechanism of the target process will help one to find simple molecular descriptors that can be calculated by cheap methods in large scale.

We outline the problems in which multireference treatment is necessary, give some basics of the CASSCF and XMCQDPT methods, and demonstrate the application of multireference computational methods to the problems of light emission, charge and energy transfer, and chemical stability of typical OLED materials.

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