

Theoretical Spectroscopy of Inner-Shell Electronic Processes and Photochemistry of Fluorescent Molecules

Masahiro Ehara and Hiroshi Nakatsuji

Abstract The SAC-CI method has been applied to the theoretical spectroscopy of the inner-shell electronic processes and the photochemistry of the organic light-emitting diodes (OLED) and biological chemosensors. Wide varieties of the core-electronic processes such as core-electron ionizations, shake-up satellites, vibrational excitations, valence–Rydberg coupling, and its thermal effect have been investigated by the SAC-CI calculations. The method has also been applied to the electronic spectra and the excited-state dynamics of the polymer materials of OLED such as poly *para*-phenylene vinylene and fluorene-thiophene. The photochemistry of the biological chemosensor has been elucidated in particular for the photo-induced electron transfer mechanism of the acridine-type fluorescent probe.

Keywords: SAC-IC · Theoretical spectroscopy · Inner-cell electronic processes · Organic-light emitting diodes · Priological chemosensors

1 Introduction

Recently, investigations of the core-electronic processes invoked renewal of interest, because significant developments in both high-resolution soft X-ray spectroscopy and accurate state-of-the-art theoretical methods have made us possible to obtain precise knowledge of the core-electronic processes. One can observe vibrational structures in the core-level photoelectron spectrum and thereby discuss the excited-state dynamics. This situation has motivated intensive cooperative researches on the core-electron processes from the experimental and theoretical sides.

Masahiro Ehara (✉)

Institute for Molecular Science, 38 Nishigo-Naka, Myodaiji, Okazaki 444-8585, Japan; JST, CREST, Sanboncho-5, Chiyoda-ku, Tokyo 102-0075, Japan, e-mail: ehara@ims.ac.jp

Hiroshi Nakatsuji

Quantum Chemistry Research Institute, Kyodai Katsura Venture Plaza 106, Kyoto 615-8245, Japan; JST, CREST, Sanboncho-5, Chiyoda-ku, Tokyo 102-0075, Japan, e-mail: h.nakatsuji@qcri.or.jp

