第320回触媒化学研究センターコロキウム
＜第2部＞

CRC

Local Coupled-Cluster Methods for Chemical Reaction Pathways Involving Large Molecular Systems

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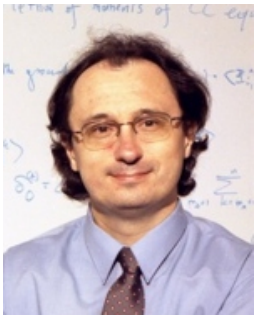

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（創成科学研究棟4階セミナー室A）
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Coupled-cluster (CC) theory has become the de facto standard for high accuracy molecular calculations, but as all electronic structure approaches that aim at the accurate description of many-electron correlation effects, it faces a number of challenges. Among them are the prohibitive costs of CC calculations for larger molecular systems. To address this challenge, we have extended a number of CC methods, including the conventional CCSD and CCSD(T) approximations, and CR-CC(2,3), which is known to provide an accurate description of chemical reaction profiles involving single bond breaking and biradicals, to larger systems with hundreds of atoms through the use of the local correlation, cluster-in-molecule (CIM) ansatz. Performance of the CIM-CC approaches and their multi-level extensions, which combine higher-level CC methods, such as CR-CC(2,3), to treat, for example, the reactive part of the large molecular system with the lower-order local or (when affordable) canonical *ab initio* schemes (e.g., MP2 or CCSD) to handle chemically inactive regions in applications involving reaction profiles will be illustrated by examining bond dissociation curves in normal alkanes and alkyl radicals, diffusion of atomic oxygen on the silicon surface, proton transfer in the aggregates of dithiophosphinic acids with the water molecules, and cobalt-methyl bond dissociation in methylcobalamin.

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Prof. Piotr Piecuch, University Distinguished Professor, Professor of Chemistry. Elected Fellow of the American Association for the Advancement of Science (2011); Elected Fellow of the American Physical Society (2008); Elected Member of the European Academy of Arts, Sciences, and Humanities (Paris, France; 2003); Professor S.R. Palit Memorial Lecturer at the Indian Association for the Cultivation of Science (2007); Profesor Catedratico Visitante at the University of Coimbra (2006); Invited Fellow of the Japan Society for the Promotion of Science and Visiting Professor at Kyoto University (2005); QSCP Promising Scientist Prize of Centre de Mecanique Ondulatoire Appliquee (France, 2004); Alfred P. Sloan Research Fellow (2002−2004); Wiley−International Journal of Quantum Chemistry Award (2000); The Polish Chemical Society Award for Research (1992, 1986)