

Preface

Theoretical and computational sciences have become one of the most exciting areas of research. For example, the Nobel Prize in chemistry in 2013 was awarded to three theoretical chemists, Professors Martin Karplus, Michael Levitt and Arieh Warshel whose works have greatly influenced many scientists and engineers. The activity at the DV- $X\alpha$ annual meeting to discuss computational sciences has continued for more than 25 years after the establishment of the DV- $X\alpha$ society in Japan and Korea. The DV- $X\alpha$ method has been utilized in not only the fundamental sciences such as physics and chemistry but also in a broader range of engineering areas such as metallurgy, material engineering, electricity, amorphous materials, photology, universology, bio-engineering, and pharmacology. This proceedings volume, entitled *The DV- $X\alpha$ Molecular-Orbital Calculation Method* is published in commemoration of the international symposium of the “Sixth International Conference on the DV- $X\alpha$ Method (DV- $X\alpha$ 2010) and The 23rd DV- $X\alpha$ Annual Meeting” held in Daejeon, KBSI, Korea, in 2010. In this volume there are 14 most powerful and interesting papers reported as recent activities involving the DV- $X\alpha$ method. Aspects of the fundamental sciences, including details of calculation methods and related programs, fundamental calculation theories and their expressions, and inter-atomic interaction potential and total energy calculations are included. In addition, a material design method which works by means of chemical bonding, discussions of optical properties of certain materials, application examples of dye-sensitized solar cells, innovative applications of water, the creation of an electrode material for lithium secondary batteries, discussions of the lifetimes of positrons, crystal structural optimization techniques, and the mechanisms of the luminescence of metal complexes are also discussed as examples of applications of the DV- $X\alpha$ method. We are very proud to publish such a high-quality and fruitful

proceedings volume which offers discussions and examples of applications which have progressed in 4 years since the previous DV-X α international meeting held in 2010.

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