

THEORY AND APPLICATIONS OF COMPUTATIONAL CHEMISTRY - 2008

Shanghai, China 23 - 27 September 2008

EDITORS

Dong-Qing Wei
Xi-Jun Wang

Wei
Wang

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PREFACE

Since the first applications of computer in chemistry in the early 1960's, "computational chemistry" has evolved today to be at the vanguard of most advances in chemistry, material science, physics, geology, biology and medicine. Its impact on chemistry can be noted from the fact that within four decades of its existence, five of the top ten most highly cited publications in 125 years of JACS are related to computational chemistry. Apart from technical advances in computers and algorithms, the phenomenal impact of computational chemistry is also due to the dedicated and sustained efforts of a large number of individuals. In this regard, we felt that it would be befitting to organize a symposium "Theory and Applications of Computational Chemistry"(TACC) in 2008 gathering nearly all of the world's leading exponents of computational chemistry. This event also follows previous successful TACC conferences, for example, 2004 TACC conference in Korea.

The 2008 TACC was co-organized by the Shanghai Jiaotong University and International Association of Scientists in the Interdisciplinary Areas(IASIA). Indeed, it provided us an excellent opportunity to get together with some most prominent scientists in the world, to name a couple of them, Prof. Rudy Marcus, the 1992 Nobel Prize Laureate in Chemistry and Prof. Martin Karplus of Harvard University. The TACC conference is featured with a large number of plenary talks, more than 50 for the 2008. The parallel sessions covers a wide range of hot topics of computational chemistry, i.e., electronic Structure, statistical mechanics and multi-scale Issues, bioinformatics and biochemistry, materials and nano, cheminformatics and drug design, chemical modeling for a sustainable environment.

The conference is a truly successful one, highly praised by the participants, also colleagues from China Conference Online, where the conference is highlighted as a feature one of 2008, most of the talks are recorded and accessible to the general public. I believe many of the participants are very much impressed by the venue(The Songjiang New Century Grand Hotel Shanghai) and organization team of the conference. I am deeply grateful for the management team of the hotel and my assistants and students, Wu Xiujun, Cong Shang, Wang Xijun, Lei Huimin to name a few. I am so happy to see Prof. E. Clementi will host the next TACC in Italy, 2012.

I received an invitation from Maya Flikop of AIP to publish conference proceedings. The response from the invited speakers is overwhelming. We received more than 50 papers, which are carefully reviewed by experts in the fields. In the end, 30 papers have been accepted, which covered virtually all the hot topics of computational chemistry.

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