2004 Annual Meeting of Chinese Chemical Society

Special Session in Theoretical and Computational Chemistry

九十三年度化學年會 理論與計算化學研討會

Sunday, November 21, 2004

National Chung Hsing Univeristy, Taichung, TAIWAN

國立中興大學

Session Chairman Prof. Chin-Hui Yu (National Tsing Hua University, Taiwan)
游靜惠 教授 清華大學化學系

08:30-09:30 Prof. Hiroshi Nakatsuji (Kyoto University, Japan)
How SAC-CI on Gaussian03 Works in Chemistry and Biology

09:30-10:00 Prof. Shih-I Lu (Fooyin Univeristy, Taiwan)
呂世伊 教授 輔英科技大學應用化學系

10:00-10:30 **Coffee Break**

10:30-11:00 Prof. San-Yan Chu (National Tsing Hua University, Taiwan)
儲三陽 教授 清華大學化學系

11:00-12:00 Prof. Kimihiko Hirao (University of Tokyo, Japan)
A New Hybrid DFT Functional: Accurate Description of Excited States, Charge-transfer States, and van der Waals Interactions

12:00-14:00 **Lunch Break**

14:00-14:30 Prof. Dah-Yen Yang (IAMS, Academia Sinica, Taiwan)
楊大衍 教授 中央研究院原子與分子科學研究所

14:30-15:00 Prof. Cheng-Lung Chen (National Sun Yat-Sen University, Taiwan)
陳正隆 教授 中山大學化學系

15:00-15:30 **Coffee Break**

15:30-17:00 Dr. Jen-Shiang K. Yu (National Chiao Tung University, Taiwan)
尤禎祥 博士 交通大學生物科技學系

Technical Workshop on Computational Chemistry

1. Optimized PC-Linux Configurations for Theoretical Calculation
2. Discussion on Computational Packages

Introduction to plenary speakers:

Prof. Hiroshi Nakatsuji was born in 1943. He completed his phD in Kyoto University, and is currently Chemistry Professor as well being the Director of Fukui Institute for Fundamental Chemistry in Kyoto University. Prof. Nakatsuji received Physical Chemistry Award of the Chemical Society of Japan in 1991, and Chemical Society of Japan Award in 2004. He has published approximately 300 research papers, including the topics in force concept for molecular geometry, theory for the direct determination of density matrix, electronic mechanism and relativistic effect in NMR chemical shifts, as well as methods of solving Schrödinger equation by providing iterative configuration interaction and extended coupled cluster formalisms. Prof. Nakatsuji's contribution in the symmetry adapted cluster configuration interaction (SAC-CI) is a highly accurate theory to study the excited states for the spectroscopy, photochemistry and molecular biology. This method has been implemented in Gaussian 03 package. The information of his laboratory and publication list is available at:
http://quanta.synchem.kyoto-u.ac.jp/english/indexe.html.

Prof. Kimihiko Hirao was born in 1945. He also received his phD in Kyoto University. He is Professor in Applied Chemistry department, and concurrently Dean of School of Engineering in University of Tokyo. Prof. Hirao was elected as the board member of International Academy of Quantum Molecular Science, of WATOC, and of International Society of Theoretical Chemical Physics. He serves as advisory editor of various international journals including Physical Chemistry Chemical Physics, Journal of Computational Chemistry, Theoretical Chemistry Accounts, Chemical Physics Letters, Journal of Theoretical and Computational Chemistry *etc.* His research field covers the development of Multireference Møller-Plesset (MRMP) theorem, as well as efficient and reliable relativistic molecular theory by two-component RESC with higher-order Douglas-Kroll (DK) Hamiltonians, which can be incorporated into *ab initio* and DFT methods. Prof. Hirao's recent work in parameter-free exchange and one-parameter correlation functionals is able to satisfy the physical requirement of specific chemical systems. His research information and list of 150 publications can be obtained at http://www.chem.t.u-tokyo.ac.jp/appchem/labs/hirao/staff/hirao/hirao.html.

Technical Workshop on Computational Chemistry:

In the lecture, the performance of programs in computational chemistry compiled by various configurations of compilers and numerical libraries on PC-Linux platforms are demonstrated. These results are additionally correlated with SPEC CPU2000 floating-point benchmark. According to the evaluation the most optimized configurations for computational chemistry in PC-Linux systems are concluded. The topics of free discussion include, but are not limited to the experiences in Linux for scientific computing, setup and management of clusters, performance tuning, and problems in theoretical calculations.

計算化學的軟體在 PC-Linux 的環境下使用不同的程式編譯器與數值函式庫會對浮點效能產生可觀的影響。經由系統化的評估程序，可以找出最佳運算效能的執行環境；同時與工業標準的 benchmark 軟體(SPEC CPU2000) 浮點測試結果作比較，可以得到完全的相關性。交流討論的主題包括但不限於 Linux 平台上的效能最佳化與計算經驗分享、叢集工作站系統的架設與管理、以及計算化學相關的各種問題等。

The above information is available in alternative formats in case of font problems at http://oxygen.chem.nthu.edu.tw/2004CCS_TCC

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