

## Symposium 2 — Chemical Dynamics, Spectroscopy and Computational Chemistry

### Monday, 17 December 2007

**Sym 2**

<b>Technical Session</b>			<b>Page</b>
<b>Date/Time</b>	Session 1 Monday, 17 December 2007 / 11:00 – 12:15 hrs		
<b>Venue</b>	Room 303		
<b>Chair</b>	Amitabha SINHA		
<b>Sym2:01</b>	11:00 – 11:30	Dynamical Resonances in the F + H <sub>2</sub> Reaction	2:31
Keynote		<i>Xueming Yang</i>	
<b>Sym2:02</b>	11:30 – 11:45	Ultrafast Vibrational Dynamics of Small Ions in Polar Solvents Studied by Nonlinear Infrared Spectroscopy	2:31
Invited		<i>K. Ohta and K. Tominaga</i>	
<b>Sym2:03</b>	11:45 – 12:00	Cell-Matrix Interactions: At the Cross-Roads of Cell Biology and Computational Chemistry	2:31
Invited		<i>M. H. Zaman</i>	
<b>Sym2:04</b>	12:00 – 12:15	Probing Altered Base Dynamics in Mismatch DNA by Time-Resolved Fluorescence Spectroscopy	2:32
		<i>Nabanita Nag, B. J. Rao and G. Krishnamoorthy</i>	

Lunch Break	12:15 – 14:00 hrs
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<b>Technical Session</b>			<b>Page</b>
<b>Date/Time</b>	Session 2 Monday, 17 December 2007 / 14:00 – 15:30 hrs		
<b>Venue</b>	Room 303		
<b>Chair</b>	Richard WONG		
<b>Sym2:05</b>	14:00 – 14:30	Theoretical Studies of Chemical Reactions — From Gas Phase Reactions to Nano Structures, Catalysts, and Enzymatic Reactions	2:32
Keynote		<i>K. Morokuma</i>	
<b>Sym2:06</b>	14:30 – 14:45	An <i>ab initio</i> Study of Ground State MH <sub>2</sub> , HMHe <sup>+</sup> and MHe <sub>2</sub> <sup>2+</sup> , M = Mg, Ca	2:32
Invited		<i>Alister J. Page and Ellak I. von Nagy-Felsobuki</i>	
<b>Sym2:07</b>	14:45 – 15:00	Quantum Chemical Simulation on Reactions in Aqueous Solution	2:33
Invited		<i>M. Aida</i>	

*Technical Program*

- Sym2:08** 15:15 – 15:30 Computational Study of Proton Transfer and Free Radical Dehydrogenation on DNA Bases: Hartree-Fock, Density Functional Theory, and Car-Parrinello Molecular Dynamics Studies 2:33  
*M. A. Martoprawiro, B. Prianto and F. Rahman*

Coffee Break	15:30 – 16:00 hrs
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<b>Technical Session</b>	Session 3	
<b>Date/Time</b>	Monday, 17 December 2007 / 16:00 – 16:45 hrs	
<b>Venue</b>	Room 303	
<b>Chair</b>	Keiji MORUKUMA	
		<b>Page</b>
<b>Sym2:09</b>	16:00 – 16:15 Mechanisms for Atmospheric Hydroxyl Radical Production Through Absorption of Long Wavelength Solar Radiation 2:33 <i>Amitabha Sinha</i>	
Invited		
<b>Sym2:10</b>	16:15 – 16:30 Nonlinear Effects in Electrokinetic Separation of Charged Macromolecules in Nanochannels 2:34 <i>S. Das, S. Duttaroy and S. Chakraborty</i>	
<b>Sym2:11</b>	16:30 – 16:45 First Principles NMR Calculations by Fragmentation 2:34 <i>A. M. Lee and R. P. A. Bettens</i>	

**Tuesday, 18 December 2007**

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<b>Technical Session</b>	Session 4	
<b>Date/Time</b>	Tuesday, 18 December 2007 / 14:00 – 15:00 hrs	
<b>Venue</b>	Room 303	
<b>Chair</b>	YANG Xueming	
		<b>Page</b>
<b>Sym2:13</b>	14:00 – 14:30 Millimeter-Wave Spectroscopy of Transient Species with Supersonic Jet Technique and UV Photolysis 2:34 <i>Keiichi Tanaka</i>	
Keynote		
<b>Sym2:14</b>	14:30 – 14:45 HOCO Radical Chemistry 2:35 <i>Joseph S. Francisco, Hua-Gen Yu and James T. Muckerman</i>	
Invited		
<b>Sym2:15</b>	14:45 – 15:00 Reactivity of the $(\eta^6\text{-C}_6\text{H}_5\text{R})\text{Cr}(\text{CO})_2\text{-}(\eta^2\text{-C}_6\text{H}_5\text{R})$ Complexes: A Laser Flash Photolysis Study 2:35 <i>Ashfaq Bengali</i>	
Invited		

Coffee Break	15:30 – 16:00 hrs
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<b>Technical Session</b>	Session 5	
<b>Date/Time</b>	Tuesday, 18 December 2007 / 16:00 – 17:00 hrs	
<b>Venue</b>	Room 303	
<b>Chair</b>	Keiichi TANAKA	
		<b>Page</b>
<b>Sym2:16</b>	16:00 – 16:30 Design of Chromogenic Anion Sensors: A Computational Approach 2:35 <i>Richard M. W. Wong</i>	
Keynote		

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<b>Sym2:17</b>	16:30 – 16:45	Time-Resolved Spectroscopic Investigation of the Reactions and Mechanisms of Phototrigger Compounds	2:36
Invited		<i>D. L. Phillips, C. Ma, W. M. Kwok, Y. Du, W. S. Chan, P. Zuo and H. Y. An</i>	
<b>Sym2:12</b>	16:45 – 17:00	Towards First Principles Molecular Dynamics of an Enzyme + Substrate	2:34
		<i>R. P. A. Bettens and A. M. Lee</i>	

### Wednesday, 19 December 2007

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<b>Technical Session</b>	Session 6 (Combine Session with Symposium 3)		
<b>Date/Time</b>	Wednesday, 19 December 2007 / 16:45 – 17:00 hrs		
<b>Venue</b>	Room 304		
<b>Chair</b>	XU Qing Hua		
	<b>Page</b>		
<b>Sym2:18</b>	16:45 – 17:00	Generalized Phase Behavior of Small Molecules and Nanoparticles	2:36
		<i>Guangwen He, Reginald B. H. Tan, Paul J. A. Kenis and Charles F. Zukoski</i>	

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<b>Technical Session</b>	Poster Session		
<b>Date/Time</b>	Wednesday, 19 December 2007 / 14:00 – 15:30 hrs		
<b>Venue</b>	Gallery		
	<b>Page</b>		
<b>Sym2:19</b>		FTIR Studies of Bromine Reaction with Methanol	2:36
		<i>J. Yang and W. Y. Fan</i>	
<b>Sym2:20</b>		A Computational Study of a Bicyclic Cyclophane Nitrate Receptor	2:37
		<i>Huifang Xie and Ming Wah Wong</i>	
<b>Sym2:21</b>		Applying Fluorescence Correlation Spectroscopy in Living Zebrafish Embryos	2:37
		<i>X. Shi, V. Korzh and T. Wohland</i>	
<b>Sym2:22</b>		Computational Study of the New SOMO Activation Model	2:37
		<i>Hui Yang and Ming Hua Wong</i>	
<b>Sym2:23</b>		A Comparative Study of Antioxidant Activities Using Coloured Free Radical Scavenging Method	2:38
		<i>Seyedeh Fatemeh Seyedreihani and Lai Peng Leong</i>	
<b>Sym2:24</b>		Investigation of Lipid-Peptide Interaction Using Fluorescence Correlation Spectroscopy	2:38
		<i>L. Guo, B. Ho, J. L. Ding and T. Wohland</i>	
<b>Sym2:25</b>		Organometallic Compounds for Cell Imaging in the Infrared	2:38
		<i>Kien Voon Kong, Moawia O. E. Ahmed, Wee Chew, Lina H. K. Lim, Wai Yip Fan and Weng Kee Leong</i>	
<b>Sym2:26</b>		Conjugated Polymer Induced Cooperative Quenching with Enhanced Selectivity Between Single- and Double-Stranded DNA	2:38
		<i>Ning Tian, Xinsheng Ren and Qing-Hua Xu</i>	
<b>Sym2:27</b>		Metal Enhanced Fluorescence of Chromophores in Core-Shell Nanocomposites	2:39
		<i>Lee Yih Hong, Daming Cheng, Manoj Parameswaran and Qing-Hua Xu</i>	
<b>Sym2:28</b>		Interactions Between a Photosensitizer and its Pharmaceutical Preparations Revealed by Fluorescence Correlation Spectroscopy	2:39
		<i>J. Liu, C. L. L. Saw, M. Olivo and T. Wohland</i>	

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## Technical Program

<b>Sym2:29</b>	Ab initio Study of Small Fe, Co & Ni Clusters on Graphene <i>H. D. S. Johll, E. S. Tok and H. C. Kang</i>	2:39
<b>Sym2:30</b>	Electronic Structure and Spectroscopy of ( <sup>1</sup> A <sub>1</sub> )MgH <sub>2</sub> <sup>2+</sup> <i>A. J. Page and E. I. von Nagy-Felsobuki</i>	2:40
<b>Sym2:31</b>	Kinetic and Equilibrium Studies of $\sigma$ -Adduct Formation and Elimination in the Reactions of 4-Nitrobenzofurazn Derivatives with Nitroalkane Anions <i>B. Asghar and M. Crampton</i>	2:40
<b>Sym2:32</b>	Why is Indigo Stable Over 100 Years? Direct Observation of Breaking and Reformation of Bonds <i>I. Iwakura, A. Yabushita and T. Kobayashi</i>	2:41
<b>Sym2:33</b>	In-Situ Interferometric Observation of Solute Diffusion Field During Directional Growth of Ice Crystals in Water-Trehalose Solution <i>Masato Suzuki and Kazushige Nagashima</i>	2:41
<b>Sym2:34</b>	Structure and Dynamics of Ice Surface <i>Tomoko Ikeda-Fukazawa</i>	2:41
<b>Sym2:35</b>	Structural Changes of Water in Poly-N,N,-Dimethylacrylamide Hydrogel During Dehydration Process <i>Y. Sekine and T. Ikeda-Fukazawa</i>	2:42
<b>Sym2:36</b>	Structure-Property Studies on the Antioxidant Activity of Three Flavon-3-ols <i>Yong Qin Chang, Kun Liu, Dou Chang and Lian Sai Chia</i>	2:42
<b>Sym2:37</b>	Photoinduced Hydrogen Atom Transfer of Tert — Butyl Radical Trapped in Low-Temperature Solid: ESR and DFT Study <i>T. Takada, H. Kawabata and H. Tachikawa</i>	2:43
<b>Sym2:38</b>	Cooperative Effects on Hydrogen Bonding of HCN-H <sub>2</sub> O-HCN Trimer: ab initio Molecular Orbital Study <i>S. Ohshita and T. Takada</i>	2:43
<b>Sym2:39</b>	Density Functional Theory Calculation for the Diatomic Molecules Adsorption on Graphite <i>Rahmat Gunawan, Muhamad A. Martoprawiro, Hermauwam K. Dipojono and Cynthia L. Radiman</i>	2:44
<b>Sym2:40</b>	Competitive Binding of Acetylsalicylic Acid and Linoleic Acid to Bovine Serum Albumin <i>B. Bojko, A. Sułkowska, M. Maciążek-Jurczyk, J. Równicka, I. Zubik-Skupień and W. W. Sułkowski</i>	2:44
<b>Sym2:41</b>	Spectroscopic Analysis of MTX-SA Complex in Rheumatoid Therapy. Comparative Study <i>M. Maciążek-Jurczyk, A. Sułkowska, B. Bojko, J. Równicka, I. Zubik-Skupień and W. W. Sułkowski</i>	2:44
<b>Sym2:42</b>	Hematoporphyrin Interaction with Serum Albumin Studied by Spectrofluorescence <i>A. Sułkowska, L. Sułkowski, A. Sieroń, M. Maciążek-Jurczyk, B. Bojko and J. Równicka</i>	2:45
<b>Sym2:43</b>	The Binding Affinity of Chemically Destabilized Defatted Human Serum Albumin Towards Sulfasalazine <i>J. Równicka, A. Sułkowska, J. Pożycka, I. Zubik-Skupień, B. Bojko, M. Maciążek-Jurczyk and W. W. Sułkowski</i>	2:45

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<b>Sym2:44</b>	Adsorption and Reaction of H <sub>2</sub> S on Clean TiO <sub>2</sub> Anatase (101) and TiO <sub>2</sub> -Rutile (110) Surfaces by First-Principles Calculations <i>Wen-Fei Huang and M. C. Lin</i>	2:45
<b>Sym2:45</b>	Novel Unsymmetrical Mononuclear Vanadium(IV) — Salicyldimine Complexes <i>Sajjad Mohebbi and Behnaz Bakhshi</i>	2:46
<b>Sym2:46</b>	Direct Observation of Time Dependent Molecular Vibration in Stilbene Derivative <i>A. Colonna, A. Yabushita, I. Iwakura and T. Kobayashi</i>	2:46
<b>Sym2:47</b>	Adsorption Configurations and Reactions of Boric Acid (B(OH) <sub>3</sub> ) on TiO <sub>2</sub> Anatase (101) Surface <i>P. Raghunath and M. C. Lin</i>	2:47
<b>Sym2:48</b>	Theoretical Investigations on the Electronic and Vibronic Spectra of Cycl[3.2.2]azines <i>Yasuhiro Shigemitsu, Takashi Kato and Tokio Yamabe</i>	2:47
<b>Sym2:49</b>	A Kinetic and Mechanistic Study of Oxidation of N-Propylamine and N-Butylamine by Chloramine-T and Chloramine-B in Aqueous Sodium Hydroxide Medium <i>M. K. Veeraiah, A. S. Ananda Murthy and N. M. Made Gowda</i>	2:47
<b>Sym2:50</b>	Calculation of Transport Properties for the Some Binary Mixtures of Light Hydrocarbons Using the Semi-Empirical Inversion Method <i>Hamid Reza Rafiee and Ramisa Esmaili</i>	2:48
<b>Sym2:51</b>	Catalytic Role of Protic Solvent in SN <sub>2</sub> Reaction: Contact Ion Pair Mechanism <i>Young-Ho Oh, Doo-Sik Ahn, Sangyoon Chung, Jeong-Hwan Jeon, Sung-woo Park, Seung Jun Oh, Dong Wook Kim, Dae Yoon Chi and Sungyul Lee</i>	2:48
<b>Sym2:52</b>	Tautomerization of Adenine Facilitated by Water: Computational Study of Microsolvation <i>Ho-Sung Kim, Doo-Sik Ahn, Sang-Yoon Chung, Joo-Young Kim, Sang Kyu Kim and Sungyul Lee</i>	2:48
<b>Sym2:53</b>	Capacitive and Piezo-Resistive Microcantilever-Based Biosensor for Biomolecular Interaction <i>Jun-Hyeok Kim, Seung-Ryong Joung, Tae-Sik Yoon, Hyun Ho Lee, C. J. Kang and Yong-Sang Kim</i>	2:48
<b>Sym2:54</b>	Preparation of Anti-Cancer Phosphoramides <i>Abdollah Javidan and Mehdi Jalalifar</i>	2:49
<b>Sym2:55</b>	An ab initio Study on Oxidative Coupling of Methane Over Titanium Oxide Catalyst <i>M. Gharibi and B. Honarparvar</i>	2:49
<b>Sym2:56</b>	Theoretical Determination of Spectroscopic Constants for Rare Gas van der Waals Complexes <i>Mahtab Gharibi and Reza Islampour</i>	2:49
<b>Sym2:57</b>	Insoluble Polynuclear Vanadyl Schiff Base Complexes <i>Sajjad Mohebbi and Maryam Abdi</i>	2:50

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