Scientific and Social Programme of QSCP-XVI - Kanazawa, Japan - September 11-17, 2011

Sunday 11/09	Monday 12/09	Tuesday 13/09		Wednesday 14/09	Thursday 15/09		Friday 16/09	Saturday 17/09
	Session CMQC-1 ***Chair: Nakatsuji***	***Session MSDS-3*** ***Chair: Hirao***		***Session RCCR-2*** ***Chair: Karlsson***	***Session CCSI-3*** ***Chair: Champagne***		***Session MNEB-1*** ***Chair: Ria Broer***	***Session CCPB-2*** ***Chair: Maruani***
	09:20 - **P. Piecuch**	09:20 - **Ria Broer**		09:20 – **W. Allen**	09:20 - **G. Delgado-Barrio**		09:20 - **K. Ruud**	09:20 - **Nakatsuji**
	09:50 - **E. Gross**	09:50 - **Yasuteru Shigeta**		09:50 - **S. Maeda**	09:50 - **Kechen Wu**		09:50 – **T. Oda**	09:50 - **Jing Ma**
	10:15 - **M. Quack**	10:15 - **Stuart Althorpe**		10:15 - **Tachikawa**	10:15 - **Hamid Berriche**		10:15 - **B. Kirtman**	10:15 - **Hanongbua**
	10:40 Coffee	**10:40 Coffee**		**10:30 Coffee**	**10:30 Coffee**		**10:30 Coffee**	**10:30 Coffee**
	Session MSDS-1 ***Chair: Brändas***	***Session CMQC-3*** ***Chair: Piecuch***		***Session CCSI-2*** ***Chair: Delgado B.***	**Session RCCR-3** **Chair: *Ruud***		***Session CCPB-1*** ***Chair: Ortiz***	***Session MNEB-2*** ***Chair: Kirtman***
	11:10 - **C. Aikens**	11:10 - **Vincent Ortiz**		11:10 - **J. S. Tse**	11:10 - **Eric Karlsson**		11:10 - **Nagaoka**	11:10 - **Z. Havlas**
	11:40 - **A. Tadjer**	11:40 - **Miroslav Urban**		11: 40 - **F. Castet**	11: 40 - **Petr Carsky**		11: 40 - **Yamanaka**	11:40 - **Chao. Hsu**
	12:05 - **O. Prezhdo**	12:05 - **S. Miura**		12: 05 – **J. Maruani**	12: 05 - **Koichi Ohno**		12: 05 – **R.Vianello**	12: 05 -
	12:30 Lunch	12:30 – **K. Hirao**	**12:40 Lunch**	**12:30 Lunch**	**12:30 Lunch**		**12:30 Lunch**	**12:30 Lunch**
	Session CMQC-2 ***Chair: Maruani***	***Session CCSI-1*** ***Chair: Aikens***	***Session AMSF-1*** ***Chair: A. Wilson***		***Session DVXa*** ***Chair: J. K awai***	***Session AMSF-3*** ***Chair: Ohno***	***Session RCCR-4*** ***Chair: Althorpe***	
15:30 and onwards	14:00 - **R. Lindh**	14:00 - **Shuhua Li**	14:00 - **Sheng Lin**		14:00 - **L. Udvardi**	14:00 - **G. Pestka**	14:00 - **Champagne**	
	14:30 - **R. Cammi**	14:30 - **M. Otani**	14:30 - **Lablanquie**		14:30 - **Mukoyama**	14:30- **Nakashima**	14:30 - **M. Nakano**	**14:30 - Closing ceremony**
Arrivals / Registration	14:55 - **Kapralova**	14:55 - **Y. Kawazoe**	14:55 - **H. Kono**		14:55 - **Fukushima**	14:55 - **Visscher**	14:55 - **Sugimoto**	
(Please bring along, if possible, electronic and paper copies of your contribution)	15:20 - **J. Hasegawa**	15:20 - **M. Saito**	15:20 - **R. Hefferlin**		15:20 - **J. Yasui**	15:20 - **H. Nakai**	15:20 - **Okumura**	**15:30 and onwards**
	15:45 Coffee	**15:45 Coffee**			**15:45 Coffee**		**15:45 Coffee**	***Departures***
	Session MSDS-2 ***Chair: Morokuma***	***Session RCCR-1*** ***Chair: Tadjer***	***Session AMSF-2*** ***Chair: Hotokka***		***Session MSDS-4*** ***Chair: Nakano***	***Session AMSF-4*** ***Chair: Nagaoka***	***Session CCSI-4*** ***Chair: Okumura***	
	16:15 - **T. Cundari**	16:15 - **Brändas**	16:15 - **A. Wilson**		16:15- **Ramasesha**	16:15 - **Fujimura**	16:15 - **B. Sutcliffe**	
	16:45 - **M. Hayashi**	16:45 - **Plakhutin**	16: 45 - **K. Yuge**		16:45 - **T. Ishii**	16:45 - **T. Kato**	16:45 - **J. Morales**	*See you next year in …*
18:00 Opening ceremony & Workshop Lecture (K. Morokuma)	17:10 - **K. Endo**	17:10 - **B. Hajgató**	17:10 - **Imamura**		17:10- **Yu Takano**	17:10 - **Kitagawa**	17:10 - **Kurokawa**	*(will be announced at the Banquet)*
19:00 Party	**15:45 To SCC**	**15:45 To SCC**		**13: 30 - *Excursion to Daizyouizi (Zene)***	**15:45 To SCC**		**15:45 To SCC**	
	Session Mo5 ***Chair:K. Endo***	**18:30 - Drum performance**		***and***	***Session Th5*** ***Chair: Oda***			
	18:15 - *25 flash poster presentations*	**19:00 - 21:00** ***Continuation of poster display***		***Sightseeing in Kanazawa***	**18:15 -** *25 flash poster presentations (3 min. each, including one to three transparencies)*		**18:30 - 20:30** ***Continuation of poster display***	
	19:30 - 21:00 ***Short snack during poster display***	*(Business meeting)*		**19:00 - *Banquet Dinner with Geiko dance and Ceremony of Award of the CMOA Prize and Medal***	**19:30 - 21:00 *Short snack during poster display***			

Poster Session 1

1. **First principle theory for the material constants**
   Marco Anelli, Dan Jonsson, Kenneth Ruud

2. **Ultrafast electronic motion in hydrogen molecular ion induced by a high power intense laser**
   H. Mineo , Y. Teranishi , S.D. Chao, and S.H. Lin

3. **Ab initio calculations of methane dimer interaction energies and molecular dynamics simulation of fluid methane**
   Arvin Huang-Te Li and Sheng D. Chao

4. **Valence XPS and Raman Spectral analysis of chitosan film modified by Kr^+ ion beam bombardments by quantum chemical calculations**
   K. Endo, H. Shinomiya, T. Ida, S. Shimada,K. Takahashi, Y. Suzuki, H. Yajima

5. **Second Hyperpolarizabilities of Open-Shell Singlet Extended Metal Atom Chains (EMACs)**
   Hitoshi Fukui, Yudai Inoue, Yasuteru Shigeta, Benoît Champagne and Masayoshi Nakano

6. **Theoretical Study on the Redox Reaction of Azurin in Water Solvent**
   Masashi Iwayama, Hiroaki Saito, Kazutomo Kawaguchi and Hidemi Nagao

7. **Blackbody, synchrotron radiation, bremsstrahlung and plasmon analyzed by Tsallis nonextensive entropy**
   Jun Kawai, Abbas Alshehabi, Hiroyuki Iwasaki, Koretaka Yuge, Ágnes Nagy

8. **Free energy of cell-penetrating peptide in lipid bilayer membrane: coarse-grained simulation**
   Shuhei Kawamoto, Takeshi Miyakawa, Masako Takasu, Ryota Morikawa, Tatsuki Oda, Hiroaki Saito, Shiroh Futaki and Hidemi Nagao

9. **Analysis for constructing protein nano-fiber including metal ions**
   Yu Komatsu, Shuhei Kawamoto, Takeshi Miyakawa, Ryota Morikawa, Masako Takasu, Satoshi Akanuma and Akihiko Yamagishi

10. **Intermonomer Interaction Effect on the Electromagnetically Induced Transparency on Molecular Aggregate Model**
    Takuya Minami and Masayoshi Nakano

11. **The potentials of the atoms around Mg^{2+} in the H-ras GTP complex and in the H-ras GDP complex**
    Takeshi Miyakawa, Ryota Morikawa, Masako Takasu, Kimikazu Sugimori, Kazutomo Kawaguchi, Hiroaki Saito and Hidemi Nagao

12. **Validation of quantum chemical methods for geometrical optimizations of sulfonamide derivatives**
Akifumi Oda, Yu Takano and Ohgi Takahashi

13. **Calculation of Energy Deposition by Swift Ions in Biomolecules: Glycine to DNA**
John R. Sabin, Stephan P. A. Sauer and Jens Oddershede

14. **Evaluation of multicenter integrals of Slater type orbitals and Coulomb-Yukawa like electric field gradient potentials using their one-range addition theorems**
Nursen SECKIN GORGUN

15. **Frank-Condon Factors for Datomic Molecules for an Arbitrary Anharmonic Potential**
L. Sandoval, I. Urdaneta and A. Palma

16. **Structural analysis of ligand binding mechanism of Hsp90**
Kazutomo Kawaguchi, Acep Purqon, Hiroaki Saito, Hidemi Nagao

17. **Antidot Structure Dependences of Open-shell Characters and Aromaticities for Hexagonal Graphene Nanoflakes**
Kyohei Yoneda, Yudai Inoue, Tomoya Inui, Yasuteru Shigeta, Takashi Kubo, Benoît Champagne and Masayoshi Nakano

Poster Session 2

1. **First-Principles Calculations of Hydrogen Impurities in Graphenes and Carbon Nanotubes**
Mohammad Shafiul Alam, Nyayu Siti Nurainun, Fahdzi Muttaqien, Agung Setiadi and Mineo Saito

2. **The potential energy surface of $Li_2^+(X^2\Sigma_g^+)$ alkali dimer colliding with the Xe atom**
S. Saidi, C. Ghanmi, F. Hassen and H. Berriche

3. **Solvation of $Li_2^+(X^2\Sigma_g^+)$ in small Xe_n clusters: structure and stability**
S. Saidi, C. Ghanmi, F. Hassen and H. Berriche

4. **Calculation of Magnetic Properties and Spectroscopic Parameters of Manganese Clusters with Density Functional Theory Methods**
Keita Kanda, Toru Saito, Yasutaka Kitagawa, Takashi Kawakamai, Shushuke Yamanaka, Kizashi Yamaguchi and Mitsutaka Okumura

5. **Ab initio and density functional calculation of calcium binding sphingomyelin lipid molecules: A pin holder model approach**
Hiroyuki Kawabe and Kimikazu Sugimori

6 **Calculation of magnetic constants D in Zero-Field Splitting by ab initio methods**

Takashi Kawakami, Keiji Kinoshita, Akira Ito, Yasutaka Kitagawa, Shusuke Yamanaka, Kizashi Yamaguchi, Mitsutaka Okumura

7. **Computational study of conformational preferences in intermediates and transition states of the hydrolysis of dimethyl phosphate**
Makoto Kita, Haruki Nakamura and Yu Takano

8 **The band 12 issue of norbornane: a comparison between symmetry adapted cluster expansion configuration interaction (SAC-CI) and the third order algebraic diagrammatic construction scheme [ADC(3)]**
S. Knippenberg and B. Hajgató

9. **Origin of the variety of the Cu_2S_2 core structure of the Cu_A sites: a density functional theory study**
Orio Okuyama, Yasuteru Shigeta, Haruki Nakamura and Yu Takano

10. **Structure and dynamics of glutathione and glutathione-transferaseT2-2: a molecular dynamics study**

Yuriko Omae, Hiroaki Saito, Kazutomo Kawaguchi and Hidemi Nagao

11. **Electronic structure calculations on vacancy-manganese center in nanodiamond systems**
Takao Otsuka, Yoshitaka Tateyama, Masahito Morita, Makoto Taiji

12. **Free energy profile of water across cholesterol containing lipid bilayer**
Hiroaki Saito and Wataru Shinoda

13. **Modifications for the electron and the polarization propagator formalisms**
Masaaki Saitow, Tomonori Ida and Yuji Mochizuki

14. **Real-Time TDDFT Simulation for Coherent Phonon Generation**
Yasushi Shinohara, Kazuhiro Yabana, Jun-Ichi Iwata, Tomohito Otobe and George F. Bertsch

15. **Theoretical study of isotope-induced additivity of chemical shift in benzene**
Kimikazu Sugimori, Hiroyuki Kawabe and Hideto Shimahara

16 **Development of First-Principles Maxwell+TDDFT Multi-Scale Simulator for Propagation of High-Intensity Laser Pulse**
Takeru Sugiyama, Yasushi Shinohara, Tomohito Otobe, Kazuhiro Yabana and George F. Bertsch

17. **Quantum Chemistry on Quantum Computers**

L. Veis and J. Pittner