

The 4th International Conference on DV-X α Method (DV-X α 2006)
and the 19th DV-X α Annual Meeting
Program

Crowne Plaza Hotel, Jeju, South Korea, 3-5 August 2006

Conference Venue: Crowne Plaza Hotel

10 minutes from Jeju Airport by bus #600 (or 5 minutes by taxi); Bus-stop at Crowne Hotel

Address: 291-30 Yeon-Dong, Jeju; 5 minutes walk from Sin-Jeju-City Rotary

Phone: 064-741-8000

www.crowneplaza.co.kr

Posters are prepared for all the speakers except for plenary speakers

All the invited speakers are also requested to present their posters. Three minutes short presentation for poster speakers should be prepared using PPT (Microsoft Office Power Point, and be saved with Main Menu > Tool(T) > Option(O) > True Type Font(E).

Or Adobe Acrobat file is also accepted. The presentation files should be saved before 13:30 on August 3rd. The file name should be Poster01.ppt, or Poster02.pdf, ... [Poster size will be announced later.](#)

August 2nd, Wednesday

The registration desk will be open from 17:00 at Crowne Plaza Hotel. From 19:00, a get-together party is scheduled; the place of the get-together party will be announced at the registration desk.

August 3rd, Thursday

Chair: Y. S. Kim

9:00 Opening Ceremony (B. I. Kim, M. Morinaga)

Chair: M. Morinaga

9:30 Plenary 1. Erkki Brändas (Uppsala University): Quantum Mechanics and the Theory of Relativity

Chair:

10:10 Invited 1. Kazuyoshi Ogasawara (Kwansei Gakuin University): Current Situation and

Future Development of Discrete Variational Multielectron (DVME) Method

Industry-Academic Cooperation Talk

10:30 Invited 2. Dong-Yoon Lee, Won-Jae Lee, Jae-Sung Song, Yang-Soo Kim (Korea Electrotechnology Research Institute, Corporate R&D Center Samsung SDI): Chemical Bonding State of Iodide Adsorbed on Surface of Carbon Nanotube

10:50-11:20 Coffee Break

Chair:

11:20 Invited 3. Masahito Yoshino (Nagoya University): 1.5 μm Luminescence and Electronic Structures in Er-containing Compounds

11:40 Invited 4. Bin Song and Pei-lin Cao (Zhejiang University): Density Functional Investigation of Geometrical and Electronic Structures of Atomic Clusters

12:00 Invited 5. Y. Kowada (Hyogo University of Teacher Education): Chemical Bonding of Mobile Cations in Superionic Conductors

12:20 -13:30 Lunch

Chair: S. Matsuo, M. Morishita, M. Yoshino

13:30 Short Presentation for Posters (3 minutes each)

13:00 Poster 1. Shino Tsuboi, Akito Takashima, Tomohiko Ishii, and Genta Sakane (Kagawa University, Okayama University of Science): Controlling of the Ligand Field Splitting and the Solid State Properties of the Metal Complexes by DV- $X\alpha$ Method

13:03 Poster 2. Akito Takashima, Shino Tsuboi, Tomohiko Ishii, and Genta Sakane (Kagawa University, Okayama University of Science): Mechanism of the RGB Color in the Porphyrin Derivatives by DV- $X\alpha$ Calculation

13:06 Poster 3. Tsutomu Kurisaki and Hisanobu Wakita (Fukuoka University): Development and Performance Evaluation of Laboratory Ultra Soft X-Ray Absorption Spectrometer

13:09 Poster 4. Shinta Watanabe (Kwansei Gakuin University): First-Principles Calculation for $f^n-f^{n-1}d^1$ Transition Absorption Spectra of Trivalent Lanthanides and Actinides in LiYF_4

13:12 Poster 5. K.Sugita, M.Mizuno, H.Araki, Y.Shirai (Osaka University): Electronic Structure

and Bonding in Amorphous $Zr_{67}Ni_{33}$ and $Zr_{67}Cu_{33}$

13:15 Poster 6. M.G. Brik, K. Ogasawara (Kwansei Gakuin University): First-Principles Calculations of Optical Spectra for Transition Metal Ions in Crystals

13:18 Poster 7. Yang-Soo Kim, Ri-Zhu Yin, Wan-Wook Choi, and Sung-Soo Kim (Samsung SDI Co. Ltd.): Lithium Vanadium Oxide as Next Generation Negative Material for Advanced Li-Ion Batteries: Structure, Analysis and First-Principles Calculation

13:21 Poster 8. Yoshiki Inoue, Hisao Yamashige, Tsutomu Kurisaki, Hisanobu Wakita (Fukuoka University): Characterization of Various Tetraaza Macrocycles using X-Ray Spectroscopy

13:24 Poster 9. Kazuhiro Fujikawa, Hisashi Yoshida, Kazuyoshi Ogasawara (Kwansei Gakuin University, NEC Lighting. Co. Ltd.): First Principles Calculation of Multiplet Structures and Absorption Spectra of ns^2 -type Ions

13:27 Poster 10. Young-Ah Jeon, Yang-Soo Kim and Kwangsoo No (Korea Advanced Institute of Science and Technology, Korea Basic Science Institute): Theoretical Study of Lithium Intercalation in Titanium Sulfides and Titanium Oxides

13:30 Poster 11. Ryusuke Teramoto, Hidenari Kai, Shinta Watanabe, Hisashi Yoshida, Kazuyoshi Ogasawara (Kwansei Gakuin University): First-Principles Calculation of Multiplet Structures of Ln^{3+} in $YAl_3(BO_3)_4$

13:33 Poster 12. Yoshifumi Shinzato, Kenji Komiya, Yoshitaka Takahashi, Hiroshi Yukawa, Masahiko Morinaga, and Shinichi Orimo (Nagoya University, Tohoku University): Characteristics of Chemical Bond in Perovskite-Type Hydrides for Hydrogen Storage

13:36 Poster 13. Satoshi Ueda and Yasuji Muramatsu (University of Hyogo): Soft X-Ray Emission Spectral Analysis of Graphite Fluoride $(CF)_n$ using DV- $X\alpha$ Calculations

13:39 Poster 14. Hironori Kawanishi, Keisuke Ishizumi, Isao Takahashi, Hikaru Terauchi, Yoshinori Hayafuji (Kansei Gakuin University): Electronic Structure Calculation of $ATiO_3$ Perovskite Oxides (A=Ba, Sr and Pb)

13:42 Poster 15. Keisuke Ishizumi, Hironori Kawanishi, Ryo Nakao, Isao Takahashi, Hikaru Terauchi, Kaoru Miura, Yoshinori Hayafuji (Kansei Gakuin University): Particle Size and Surface Effects on Critical Thickness for Ferroelectricity of $BaTiO_3$ by First-Principles Calculation

13:45 Poster 16. Sung Kwan Kim, Yang-Soo Kim and Kwangsoo No (Korea Advanced Institute of Science and Technology): The Electronic Structures and Optical Properties of Hf-O-N Thin Films as a Phase Shift Mask for ArF Laser Lithography

13:48 Poster 17. Yoshitsune Higashiguchi, Hiroaki Ochiai, Kazuyuki Igei, Yoshinori Hayafuji (Kansei Gakuin University): Theoretical Study of the Stability of XB_{12} and XB_6 Clusters, $X=H-Br$

13:51 Poster 18. Koichi Nakagawa, Setsuko Matsumoto and Hironaga Matsumoto (Meiji University): Analysis of VUV Reflection Spectra of KDP, RDP and KDA by DV- $X\alpha$ Method

13:54 Poster 19. Yusuke Kinoshita, Atsushi Nakamura, Takayuki Noguchi, Takeshi Inoue, Takumi Tomita and Yoshinori Hayafuji (Kansei Gakuin University): Electronic Structures of ZnO Doped by Various Atoms (from Li to Bi without Radioactive Atoms)

13:57 Poster 20. Sunao Sugihara, Shunsuke Naitoh, Koujiroh Nishiyama, Yuka Igarashi and Kentaroh Morikawa: Thermoelectric Properties of the Oxide and Electronic Structures

14:00 Poster 21. Takeshi Mukoyama (Kansai Gaidai University): Chemical Effect on $K\beta/K\alpha$ X-Ray Intensity Ratios for Potassium Compounds

14:03 Poster 22. Hiroshi Tsutsumi, Manabu Fuziwara, Tsutomu Kurisaki, and Hisanobu Wakita (Fukuoka University): Electronic Structure Analyze of Various Types of Lithium Compounds using an X-Ray Absorption Spectroscopic Analysis Method

14:06 Poster 23. Chikashi Suzuki, Toshio Nakagiri, and Kazumi Aoto (Japan Atomic Energy Agency): Sulfur Trioxide Adsorption on Pt Electrode

14:09 Poster 24. Shoichi Takayama, Takeshi Tanigaki, and Jun Kawai (Kyoto University): On Plasmon and Bremsstrahlung

14:12 Poster 25. Masanori Sakaguchi, Rie Endo, Masahiro Susa (Tokyo Institute of Technology): Synthesis of New Coloured Alloys Based upon Colour Specification and Density of States

14:15 Poster 26. Y. Shinzato, H. Yukawa, M. Morinaga, T. Baba and H. Nakai (Nagoya University, Waseda University): New Expression of the Chemical Bond in Hydrides Using Atomic Energy Densities

Chair: H. Yoshida, T. Ishii

Industry-Academic Cooperation Poster Session

14:18 Poster 27. Hidenari Kai, Hisashi Yoshida, Kazuyoshi Ogasawara (Kwansei Gakuin University, NEC lighting): First-Principles Calculations for Phosphorescent Molecule Ir(ppy)₃ used in Organic Light Emitting Diodes

14:21 Poster 28. M. Morinaga, Y. Murata, R.Hashizume, A.Yoshinari and T. Kiyono (Nagoya University, The Kansai Electric Power Company Inc., Hitachi Co. Ltd.): Design and Development of Ni-based Single Crystal Superalloys for Gas Turbine Blades Using the Alloying Parameters Obtained by DV-X α Method

14:24 Poster 29. Young-Ah Jeon, Sung-Kwan Kim, Yang-Soo Kim and Kwangsoo No (Korea Advanced Institute of Science and Technology, Korea Basic Science Institute): Comparison the Electronic Structures between Li(Ni_{0.5}Mn_{0.5})O₂ and Li(Ni_{1/3}Mn_{1/3}M_{1/3})O₂ (M=Al and Co) for Lithium Battery Cathode Materials

14:27 Poster 30. Masataka Mizuno, Teruo Kihara, Hideki Araki, Yasuharu Shirai, Takashi Onishi (Osaka University, Kobe Steel Ltd.): Theoretical Calculation of Positron Lifetimes of Vacancy Clusters in Cu

14:30 Poster 31. B.S. Kim, D.Y. Lee, M.W. Oh, S.D. Park, H.W. Lee, W.S. Chung, T. Ishii (Korea Electrotechnology Research Institute, Pusan National University, Kagawa University): Comparison of Electronic State Calculation and Experimental Results of Electrical Conductivity of Mn-X(transition elements) Oxide by Anodic Deposition

14:33 Poster 32. Akira Kubo, Shinta Watanabe, Hiroki Moriwake, Kazuyoshi Ogasawara (Kwansei Gakuin University, Japan Fine Ceramics Center): An Approach for Design of Magnetic Materials Based on Spinel Ferrites using First-Principles Calculations

16:40-18:00 Coffee and Poster Session

19:00 Welcome Reception

August 4th, Friday

Chair: B. I. Kim

9:00 Plenary 2. Laszlo Kövér (Institute of Nuclear Research of the Hungarian Academy of Sciences): Local Electronic Structures from Analyzing and Modeling High Energy Auger and

Photoelectron Spectra of Solids

Chair: T. Hayafuji

9:40 Invited 6. Yasuji Muramatsu (University of Hyogo): Soft X-Ray Spectral Analysis of Industrial Carbon Materials using DV- $X\alpha$ Calculations

10:00 Invited 7. Young-Min Kim, Jin-Kyu Kim, Youn-Joong Kim (Korea Basic Science Institute): Electron Spectroscopy by Energy-Filtered High Voltage Electron Microscopy

10:20-10:50 Coffee Break

Chair: J. Kawai

10:50 Invited 8. Shuji Matsuo (Kobe Steel, LTD.): X-Ray Absorption Spectroscopic Study on Polymerization of Aqueous Aluminate and Theoretical Analysis by DV- $X\alpha$ MO Method

11:10 Invited 9. Hisao Yamashige, Shuji Matsuo, Tsutomu Kurisaki, and Hisanobu Wakita (Fukuoka University): Local Structure Analyses of Nitrogen Atoms in a Porphine Ring of meso-Phenyl Substituted Porphyrin and Related Compounds with an Electron-Withdrawing Group Using X-ray Photoelectron Spectroscopy and X-ray Absorption Spectroscopy

11:30 Invited 10. Qiang MIAO, Chun-gen Liu, Hirohiko Adachi, Isao Tanaka (Nanjing University, Kyoto University): DV- $X\alpha$ Study on Quantum Mirages and Quantum Corrals in Non-Metal Systems

11:50 Invited 11. H.Yukawa, M.Maeda, M.Morinaga and S.Inoue (Nagoya University, Numazu National College of Technology): Alloying Effects on the Electronic Structures of Tungsten

12:10 Lunch

Chair: H. Wakita

14:00 Plenary 3. Yuichi Ikuhara (The University of Tokyo): Grain Boundary Atomic Structures in Oxide Ceramics

15:00 Excursion

19:00 Banquet

August 5th, Saturday

Chair: T. Mukoyama

9:00 Plenary 4. S. Nasu (Osaka University): Hyperfine interaction study of materials and related DV- $X\alpha$ calculations

Chair:

9:40 Invited 12. Masao Morishita and Hiroaki Yamamoto (University of Hyogo): Thermal Spectroscopy of $Mg_{48}Zn_{52}$, Mg_2Zn_3 , $MgZn_2$ and Mg_2Zn_{11} from Near Absolute Zero Kelvin: Electronic Term Contributing to Heat Capacity, Electric Resistivity and Thermal Conductivity

10:00 Invited 13. Tatiana Nedoseykina, Ri-Zhu Yin, Joo-Han Song and Sung-Soo Kim (Samsung SDI Co. Ltd.): Lithium Insertion/Removal Mechanism of $Li_{1.1}V_{0.9}O_2$ Negative Electrode in Lithium Ion Cell

10:20-10:50 Coffee Break

Chair: Y. Kowada

10:50 Invited 14. Kimichika Fukushima (AITEL Corporation): First-Principle Analysis of Metal Oxides and Investigation of Catalytic Properties for Dimethyl Ether Steam Reforming

11:10 Invited 15. Tomohiko Ishii, Yuya Yamaoka, Daisuke Kudo, Genta Sakane, and Masataka Mizuno (Kagawa Univ., Okayama Univ. of Sci., Osaka Univ.): Electronic Structures and Magnetic Properties of Single-Molecule Magnets (SMMs)

[Industry-Academic Cooperation Talk](#)

11:30 Invited 16. Hisashi Yoshida, and Kazuyoshi Ogasawara (NEC Lighting, Ltd, Kansei Gakuin University): A Novel Study of Phosphors using Relativistic DV- $X\alpha$ Method

Chair: J. Kawai

12:00 DV- $X\alpha$ Award Ceremony (K. Fukushima), DV- $X\alpha$ Association Assembly (M. Morinaga), and Closing Address (H. Adachi)

Non-members are welcome to attend the Assembly as an observer.

Lunch