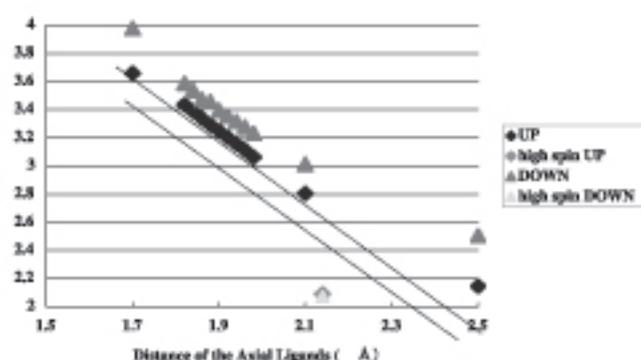
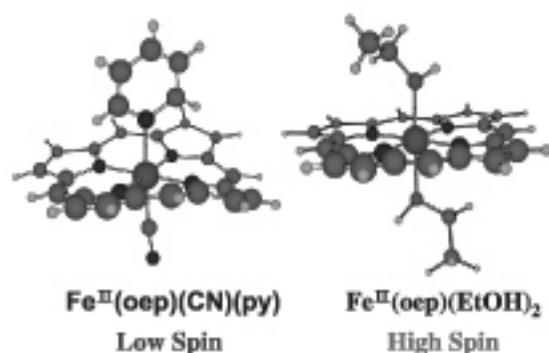


# DV- $X\alpha$ 研究協会会報

Bulletin of the Society for Discrete Variational  $X\alpha$   
Vol.19, No.1&2 (2006)

DV- $X\alpha$  研究協会会報  
Vol. 19  
No. 1 & 2  
(2006)



Axial ligand distance dependence of the field ligand splitting of the Fe(III)(por)(CN)(py) cluster model.

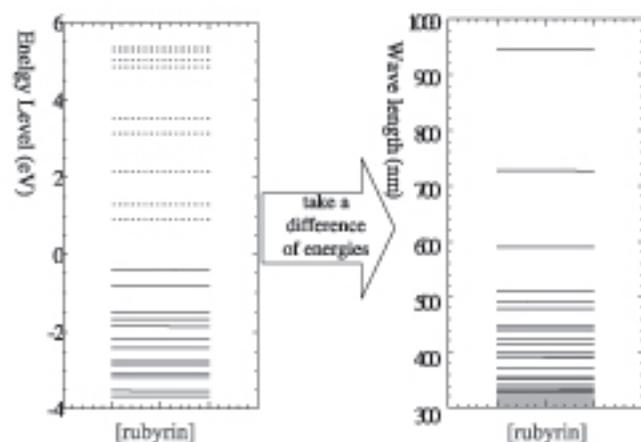
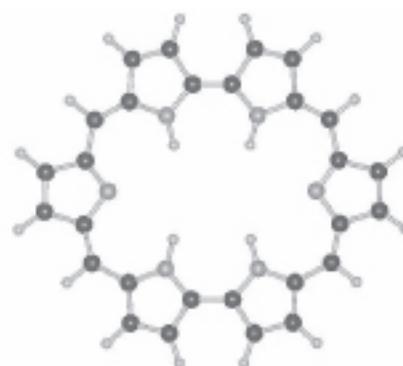


Diagram of the absorption wavelength calculation.



rubyrin: ((26)- phxaphyrin(1. 1. 0. 1. 1. 0))

# DV-X $\alpha$ 研究協会会報

Bulletin of the Society for Discrete Variational X $\alpha$   
Vol. 19, No. 1&2 (2006)

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編集 DV-X $\alpha$  研究協会

**The 4th International Conference on DV-X $\alpha$  Method (DV-X $\alpha$  2006)  
--- Industrial-Academic Cooperation Symposium  
and the 19th DV-X $\alpha$  Annual Meeting --- Program**

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

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**Conference Venue: Crowne Plaza Hotel Jeju**

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Crowne Plaza Hotel Jeju is located in the heart of Jeju City, just 5 minutes from Jeju International Airport. The most convenient way from the airport is to take a taxi, app. KRW 2500 (2.50 USD). Or 10 minutes from Jeju Airport by bus #600; Bus-stop at Crowne Hotel.

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

Hotel Phone: 064-741-8000, Hotel website: [www.crowneplaza.co.kr](http://www.crowneplaza.co.kr)

Official website: <http://dvxa.com/> and <http://dvxa.com/DVXA2006/>

Japanese website: <http://www.dvxa.org>

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**Posters are prepared for all the speakers except for plenary speakers**

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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 as Main Menu > Tool(T) > Option(O) > True Type Font(E) into USB memory. 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 board size is 1 m in width and 2 m in height. Pins, in order to put the posters, are prepared by the organizer. Poster award is scheduled (details will be announced later).

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**August 2nd, Wednesday**

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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.

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**August 3rd, Thursday**

---

**Chair: Y. S. Kim**

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

**Chair: M. Morinaga**

**9:15 Plenary 1. Erkki Brändas (Uppsala University): Quantum Mechanics and the Theory of Relativity**

**Chair: Y. J. Kim**

**9:55 Invited 1. Kazuyoshi Ogasawara (Kwansei Gakuin University): Current Situation and Future**

Development of Discrete Variational Multielectron (DVME) Method

**Industrial-Academic Cooperation Talk**

**10:15 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

**10:35-11:05 Coffee Break**

**Chair: Qiang Miao**

**11:05 Invited 3. Masahito Yoshino** (Nagoya University): 1.5  $\mu\text{m}$  Luminescence and Electronic Structures in Er-containing Compounds

**11:25 Invited 4. Tatiana Nedoseykina**, Ri-Zhu Yin, Joo-Han Song and Sung-Soo Kim (Samsung SDI Co. Ltd.): Lithium Insertion/Removal Mechanism of  $\text{Li}_{1.1}\text{V}_{0.9}\text{O}_2$  Negative Electrode in Lithium Ion Cell

**11:45 Invited 5. Bin Song** and Pei-lin Cao (Zhejiang University): Density Functional Investigation of Geometrical and Electronic Structures of Atomic Clusters

**12:05 -13:30 Lunch**

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

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

**13:30 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

**13:33 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

**13:36 Poster 3.** Tsutomu Kurisaki and Hisanobu Wakita (Fukuoka University): Development and Performance Evaluation of Laboratory Ultra Soft X-Ray Absorption Spectrometer

**13:39 Poster 4.** Shinta Watanabe, Takugo Ishii, and Kazuyoshi Ogasawara (Kwansei Gakuin University): First-Principles Calculation for  $f^n-f^{n-1}d^1$  Transition Absorption Spectra of Trivalent Lanthanides and Actinides in  $\text{LiYF}_4$

**13:42 Poster 5.** K.Sugita, M.Mizuno, H.Araki, Y.Shirai (Osaka University): Electronic Structure and Bonding in Amorphous  $Zr_{67}Ni_{33}$  and  $Zr_{67}Cu_{33}$

**13:45 Poster 6.** M.G. Brik, K. Ogasawara (Kwansei Gakuin University): First-Principles Calculations of Optical Spectra for Transition Metal Ions in Crystals

**13:48 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

**13:51 Poster 8.** Yoshiki Inoue, Hisao Yamashige, Tsutomu Kurisaki, Hisanobu Wakita (Fukuoka University): Characterization of Various Tetraaza Macrocycles using X-Ray Spectroscopy

**13:54 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

**13:57 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

**14:00 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  $YAl_3(BO_3)_4$

**14:03 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

**14:06 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

**14:09 Poster 14.** Hironori Kawanishi, Keisuke Ishizumi, Isao Takahashi, Hikaru Terauchi, Yoshinori Hayafuji (Kwansei Gakuin University): Electronic Structure Calculation of  $ATiO_3$  Perovskite Oxides (A=Ba, Sr and Pb)

**14:12 Poster 15.** Keisuke Ishizumi, Hironori Kawanishi, Ryo Nakao, Isao Takahashi, Hikaru

Terauchi , Kaoru Miura, Yoshinori Hayafuji (Kwansei Gakuin University): Particle Size and Surface Effects on Critical Thickness for Ferroelectricity of BaTiO<sub>3</sub> by First-Principles Calculation

**14:15 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

**14:18 Poster 17.** Yoshitsune Higashiguchi, Hiroaki Ochiai, Kazuyuki Igei, Yoshinori Hayafuji (Kwansei Gakuin University): Theoretical Study of the Stability of XB<sub>12</sub> and XB<sub>6</sub> Clusters, X=H~Br

**14:21 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

**14:24 Poster 19.** Yusuke Kinoshita, Atsushi Nakamura, Takayuki Noguchi, Takeshi Inoue, Takumi Tomita and Yoshinori Hayafuji (Kwansei Gakuin University): Electronic Structures of ZnO Doped by Various Atoms (from Li to Bi without Radioactive Atoms)

**14:27 Poster 20.** Sunao Sugihara, Shunsuke Naitoh, Koujiroh Nishiyama, Yuka Igarashi and Kentaroh Morikawa: Thermoelectric Properties of the Oxide and Electronic Structures

**14:30 Poster 21.** Takeshi Mukoyama (Kansai Gaidai University): Chemical Effect on K $\beta$ /K $\alpha$  X-Ray Intensity Ratios for Potassium Compounds

**14:33 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

**14:36 Poster 23.** Chikashi Suzuki, Toshio Nakagiri, and Kazumi Aoto (Japan Atomic Energy Agency): Sulfur Trioxide Adsorption on Pt Electrode

**14:39 Poster 24.** Shoichi Takayama, Takeshi Tanigaki, and Jun Kawai (Kyoto University): On Plasmon and Bremsstrahlung

**14:42 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

**14:45 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

**14:48 Poster 27.** W. Takahara and F. Minami (Osaka University): Chemical nature of Si-O bonds in silica-based clusters - Linking for element selection rules in biological system -

**Chair: H. Yoshida, T. Ishii**

**Industrial-Academic Cooperation Poster**

**14:51 Poster 28.** Hidenari Kai, Hisashi Yoshida, Kazuyoshi Ogasawara (Kwansei Gakuin University, NEC lighting): First-Principles Calculations for Phosphorescent Molecule Ir(ppy)<sub>3</sub> used in Organic Light Emitting Diodes

**Industrial-Academic Cooperation Poster**

**14:54 Poster 29.** 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 $\alpha$  Method

**Industrial-Academic Cooperation Poster**

**14:57 Poster 30.** 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<sub>0.5</sub>Mn<sub>0.5</sub>)O<sub>2</sub> and Li(Ni<sub>1/3</sub>Mn<sub>1/3</sub>M<sub>1/3</sub>)O<sub>2</sub> (M=Al and Co) for Lithium Battery Cathode Materials

**Industrial-Academic Cooperation Poster**

**15:00 Poster 31.** 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

**Industrial-Academic Cooperation Poster**

**15:03 Poster 32.** 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

**Industrial-Academic Cooperation Poster**

**15:06 Poster 33.** 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

**15:09 Poster 34.** Seigo Kishno, Koji Sueoka and Haruhiko Yoshida (Fukui University of Technology, Okayama Prefectural University, University of Hyogo): Energy band structure of strained semiconductor studied by DVX $\alpha$  calculation using madelung potential

**15:30-18:00 Coffee and Poster Session**

**19:00 Welcome Reception**

---

**August 4th, Friday**

---

**Chair: S. S. 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: Y. 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**

**13:45 Conference Photo**

**Chair: H. Wakita**

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

**15:00-19:00 Excursion**

**20:00 Banquet**

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**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: D. Y. Lee**

**9:40 Invited 12. Masao Morishita** and Hiroaki Yamamoto (University of Hyogo): Thermal Spectroscopy of Mg<sub>48</sub>Zn<sub>52</sub>, Mg<sub>2</sub>Zn<sub>3</sub>, MgZn<sub>2</sub> and Mg<sub>2</sub>Zn<sub>11</sub> from Near Absolute Zero Kelvin: Electronic Term Contributing to Heat Capacity, Electric Resistivity and Thermal Conductivity

**10:00 Invited 13. Y. Kowada** (Hyogo University of Teacher Education): Chemical Bonding of Mobile Cations in Superionic Conductors

**10:20 Invited 14. Katsumi Nakagawa** (Canon Inc.) Trial of non-LCAO DVX $\alpha$  method

**10:40-11:00 Coffee Break**

**Chair: Y. Kowada**

**11:00 Invited 15. Kimichika Fukushima** (AITEL Corporation): First-Principle Analysis of Metal Oxides and Investigation of Catalytic Properties for Dimethyl Ether Steam Reforming

**11:20 Invited 16. 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)

**Industrial-Academic Cooperation Talk**

**11:40 Invited 17. Hisashi Yoshida**, and Kazuyoshi Ogasawara (NEC Lighting, Ltd, Kwansei 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), Closing Address (H. Adachi)**

**12:15 DV- $X\alpha$  Association Assembly (M. Morinaga),**

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

Lunch

# 第 19 回 DV-X $\alpha$ 研究会報告書

## Reports of DV-X $\alpha$ 2006

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※第一著者(講演者)の名前のみしめしました。

<編集後記>

2006年度は日韓合同の国際会議ということで、No.1と2の合併号にいたしました。

ご了解をお願いいたします。

また、発行が遅れ、関係者にご迷惑をおかけすることになってしまいました。

この場を借りてお詫び申し上げます。

今号の表紙は香川大学の高嶋明人さんにお願ひしました。

会報についてのご意見は遠慮なく下記へお寄せください。

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DV-X $\alpha$ 研究協会会報, Vol. 19, No. 1&2 (2006)

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