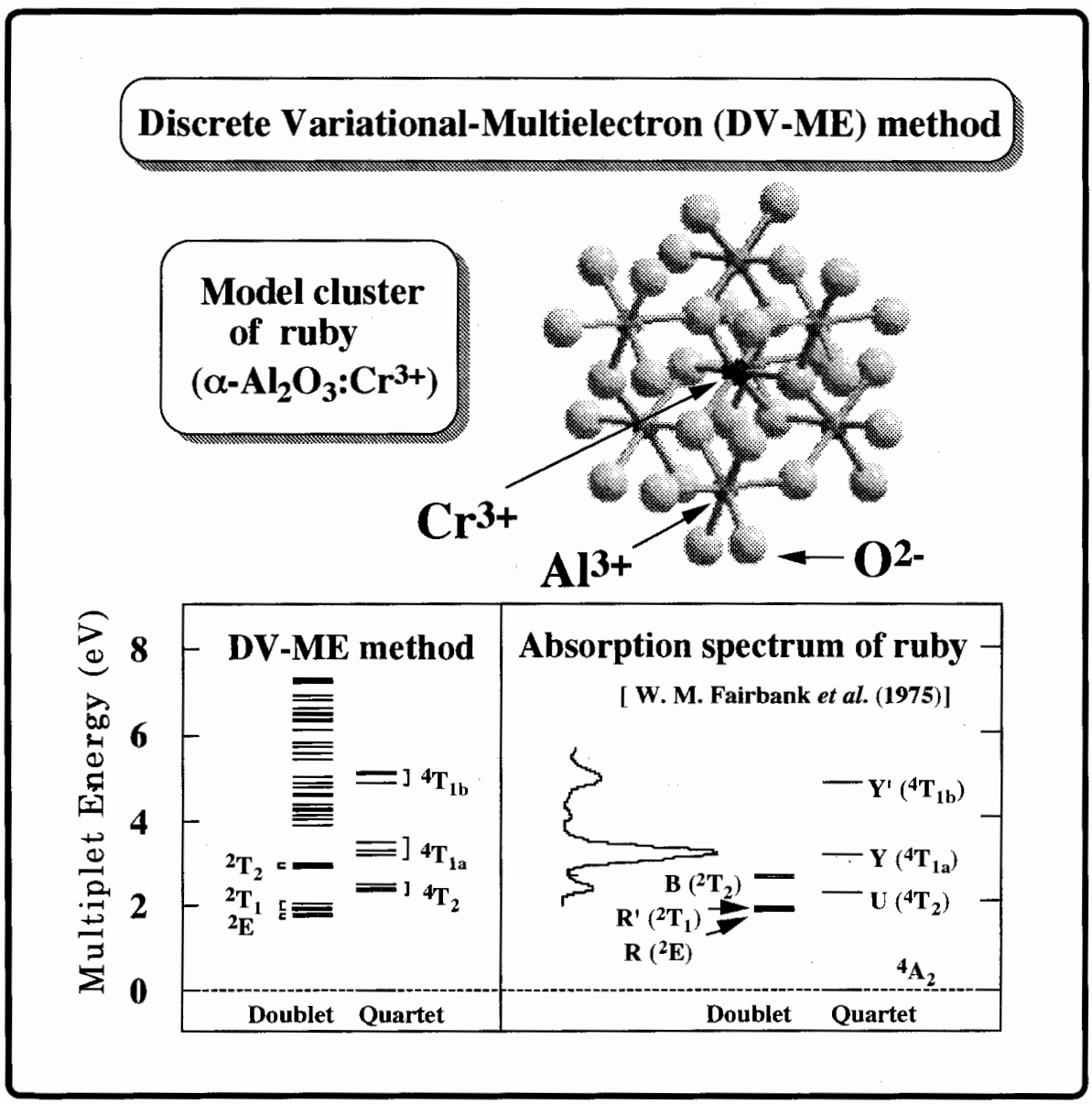
DV-Xα 研究協会会報

Bulletin of the Society for Discrete Variational Xα

Vol. 11 , No. 1 (1998)



編集　DV-Xα 研究協会

DV-Xα 研究協会会報

Bulletin of the Society for Discrete Variational Xα
Vol. 11, No. 1 (1998)

目次

編集　DV-Xα 研究協会

Korea-Japan DV-Xα Joint Symposium('98)

11th DV-X*α* *Annual Meetings*

Abstracts

DVX*α*

Aug 3-5, 1998

at Hoam Faculty House

Seoul National University

Seoul, Korea

○ Organizations

Chairperson

H. Wakita Fukuoka University
S. J. Park Seoul National University
H. Kim Seoul National University

Organizing and Scientific Committee

K. Fukushima Toshiba, Japan
M. C. Chang Kunsan National University, Korea
H. Adachi Kyoto University, Japan
M. Uda Waseda University, Japan
Y. Hayafuji Sony, Japan
H. J. Chang KRICT, Korea
Y. S. Kang Samsung Electronics, Korea
J. Kawai Kyoto University, Japan
B. K. Kim KIST, Korea
H. Kim Seoul National University, Korea
M. Morinaga Nagoya University, Japan
T. Mukoyama ICR, Kyoto University, Japan
S. Nasu Osaka University, Japan
R. Sekine Shizuoka University, Japan
T. Shbahara Okayama University of Science, Japan
J. Tanaka NIRIM, Japan
K. Taniguchi Osaka Electro-Communication University, Japan

Supported by

KOSEF(Korea)
JSPS(Japan)

August 3 (Mon.)

10:00 - 11:00 Opening Ceremony

Chairperson: Hisanobu Wakita

Fine Ceramics in Japan and Korea, Hwan Kim, Seoul National University

Progress of DV-Xα in Japan, Hirohiko Adachi, Kyoto University

Bridge between Korea and Japan in DV-Xα", Myung Chul Chang, Kunsan National University

Research by DV-Xα method in Japan,

Activity of the TANUKI meeting (the former "relativistic division")

Rika Sekine, Shizuoka University

11:00 - 11:40 "Clusters"

Chairperson: Tomoyuki Yamamoto

A1 Comparison of Boron with Aluminum Clusters

Kazuyoshi Adachi*, Rika Sekine, Shizuoka Univ.; and Jun Onoe, RIKEN

A2 Geometries and electronic structures of 3d-transition metal clusters

Ryuichi Kondo*, Kumiko Tanaka, and Rika Sekine, Dep. of Chemistry, Faculty of Sci., Shizuoka Univ.; Jun Onoe, Kazuo Takeuchi, Riken; and Hirohide Nakamatsu, Chemical Research Institute, Kyoto Univ.

A3 Electronic Structure of a Sandwich Cubane-Type Cluster with Molybdenum -Cadmium-Sulfur ($Mo_3S_4CdS_4Mo_3$) Core

Genta Sakane*, and Takashi Shibahara*, Department of Chemistry, Okayama University of Science; and Hirohiko Adachi, Department of Metallurgy, Kyoto University

A4 Local electronic states of oxygen vacancies in metal oxides

Makoto Azuma*, Shigeto R. Nishitani, Isao Tanaka, and Hirohiko Adachi, Department of Materials Science and Engineering, Kyoto University

A5 Impurity states in ZnO ceramics by cluster calculations

Fumiyasu Oba*, Hirohiko Adachi, Department of Materials Science and Engineering, Kyoto University; and Isao Tanaka, Department of Energy Science and Technology, Kyoto University

Comment

11:40 - 13:10 Lunch

13:10-13:50 "Materials Science I"

Chairperson: Jun Yasui

A6 Nature of Chemical Bonding in Sulfur Fuorides

Kumiko Tanaka*, and Rika Sekine, Dep. of Chemistry, Faculty of Science, Shizuoka University; Jun Onoe, RIKEN; and Hirohide Nakamatsu, Chemical Research Institute, Kyoto Univ.

A7 Metal-Hydrogen Interactions in Hydrogen Storage Alloys

Kenichi Nakatsuka*, Hiroshi Yukawa and Masahiko Morinaga, Department of Materials Science and Engineering, Graduate School of Engineering, Nagoya University

A8 Electronic Structures of Hydrogen in Perovskite-type Oxide, $SrZrO_3$

M.Yoshino*, K.Nakatsuka, H.Yukawa and M.Morinaga, Department of Materials Science and Engineering, Graduate school of Engineering, Nagoya University

A9 Electronic structure and chemical bonding of T_$MTiS_2$ (T_M=Cr, Fe) by cluster calculation
Yang-Soo Kim*, Isao Tanaka, and Hirohiko Adachi, Department of Materials Science and Engineering, Kyoto University

A10 Electronic Structures of Polymorphous Phases in Perovskite-type Oxide, $SrZrO_3$
H.Yukawa*, M.Yoshino and M.Morinaga, Department of Materials Science and Engineering, Graduate school of Engineering, Nagoya University

A11 The electronic structures for ferroelectricity and antiferroelectricity
M. Fujita and S. Sugihara, Shonan Institute of Technology; and R. Sekine, Shizuoka University

A12 Electronic State of AgI-based Superionic Conducting Materials
Yoshiyuki Kowada* and Yoshinobu Yamadaa, Hyogo University of Teacher Education; and Hirohiko Adachi, Department of Materials Science and Engineering, Kyoto University

Comment

13:50-14:20 Coffee Break

14:20 - 15:20 "Keynote Speech"
Chairperson: Rika Sekine

A13 Electronic Structures of Hydrogen Storage Alloys
M. Morinaga, Department of Materials Science and Engineering, Graduate School of Engineering, Nagoya University

15:20-16:00 "Dynamics"(Invited Speech)
Chairperson: Hyunju Chang

A14 Calculation of Transition Probability for Nonadiabatic Process
Jun Yasui*, Toyobo Co. Ltd. Research Center

A15 New directions in X-ray emission and absorption spectroscopy with high brightness synchrotron radiation: Theoretical challenges
Rupert C.C. Perera, Center for X-ray Optics, Lawrence Berkeley National Laboratory, Berkeley, CA 94720, USA

Comment

16:00-16:20 Coffee Break

16:20 - 17:00 "Spectroscopy I"
Chairperson: Takahiro Kaneyoshi

A16 The effect of Ti 3d core-hole on Ti L-edge ELNES for $SrTiO_3$
Nobuki Hosoi*, Silicon Systems Research Laboratories, NEC Corporation

A17 Interpretation of Si-L2,3 edge electron energy loss near edge structure (ELNES) obtained from intergranular glassy film of Si_3N_4 ceramics.
Masato YOSHIYA*, Isao Tanaka, and H. Adachi, Kyoto University

A18 Core-hole Effects on B-K edge ELNES from Boron Nitride Polytypes
Hiroyuki Araki*, Isao Tanaka, Kazuyoshi Ogasawara, and Hirohiko Adachi, Kyoto University

A19 Fine Structure Analysis of X-ray Emission and Absorption Spectra of Low-Z Elements.

[1]T.Yamamoto and [1,2]M.Uda, [1]Laboratory for Materials Science and Technology, Waseda University, [2]Department of Materials Science and Engineering, Waseda University

A20 Theoretical analysis of O Kα spectra

S. Sassa, T. Yamamoto and M. Uda, Department of Materials Science and Engineering, Waseda Univerity, 3-4-1 Okubo, Tokyo 169-8555, Japan

A21 Theoretical analysis of Kβ X-ray spectrum emitted from third-row elements

K.Hayashi, T.Yamamoto and M.Uda, Department of Material Science and Engineering, Waseda University

A22 Theoretical analysis of O-K X-ray absorption and emission spectra of Cu oxides

H.Osawa, T.Yamamoto and M.Uda, Department of Materials Science and Engineering, Waseda University

17:00 Official Comment

17:10 - 21:00 Committee

17:10 - 21:00 Poster Session

August 4

9:00-9:10 Official Comment

9:10-10:10 "Keynote Speech"

Chairperson: Sunao Sugihara

B1 CRYSTAL STRUCTURE AND GRAPH

Su Jin Chung, School of Materials Science and Engineering, Seoul National University, Seoul 151-742, Korea

10:10-10:50 "Spectroscopy II"

Chairperson: Hyunju Chang

B2 A Structural Study of Dibromo(1,4,8,11-tetraazacyclotetradecane)copper(II) Complex in Crystal and in Aqueous Solution by X-ray Absorption Near Edge Structure Measurements and DV-Xα Calculations

Shuji Matsuo*, Toshio Yamaguchi, and Hisanobu Wakita, Department of Chemistry, Fukuoka Univ.

B3 DV-Xα Analysis of N-K XANES spectra for trans- [Ni(II) L Cl2] and trans-[Cu(II) L Cl2] ,(L=1,4,8,11-tetraazacyclotetradecane)

Kenji Koga, Satoshi Kurisaki, Toshio Yamaguti and Hisanobu Wakita, Department of Chemistry, Fukuoka Univ.

B4 A XANES study on the multinuclear transition metal complexes by a DV-Xα analysis

Mitsutoshi Yokomizo*, Tsutomu Kurisaki, Toshio Yamaguchi, and Hisanobu Wakita

Department of Chemistry, Faculty of Science, Fukuoka University

B5 A structural study on the analysis of Al-K X-ray Absorption Near Edge Structure for a series of Aluminosilicate minerals
Hikoshiro Ichihashi*, Satoshi Kurisaki*, Toshio Yamaguchi* and Hisanobu Wakita*, *Department of Chemistry, Fukuoka Univ

B6 Calculation of Cu K-edge XANES for copper oxides
Minoru Ishizuka*, and Rika Sekine, Department of Chemistry, Faculty of Science, Shizuoka Univ.; and Hirohide Nakamatsu, Institute for Chemical Research, Kyoto Univ.

B7 F K Emission Spectra of Fluorides of Different Cation Coordinations
Sujin Kim and Sunja Park, School of Materials Science and Engineering, Seoul National University; Jun Kawai and Hirohiko Adachi, Department of Materials Science and Engineeing, Kyoto University

Comment

10:50 - 11:20 Coffee Break

11:20-11:40 "Invited Speech"

Chairperson: Masao Morishita

B8 Electronic structure of Ti_4O_7 using DV-Xα cluster calculation method
Hyunju Chang* and J. D. Lee, Korea Research Institute of Chemical Technology, Taejon, 305-600, Korea

Comment

B[illegible] Application of DV-Xα to the Firsov Model of Electronic Stopping Force in Slow Velocity Atomic Collisions
Masahiko KATO* ,School of Engineering, Nagoya University

11:40-13:20 Lunch

13:20-13:50 "Surface"

Chairperson: Hiroshi Yukawa

B9 Relationship between Work Function of Metals and Stacking Faults
Y. Fujimoto, A. Nakamura and M. Uda, Dept. of Materials Science and Engineering, Waseda Univ. 3-4-1 Okubo, Shinjyuku-ku, Tokyo, 169-8555, Japan

B10 Initial oxidation and hydroxydation of Al exposed to wet air
M. Kawasaki, Y. Nakagawa and M. Uda, Department of Materials Science and Engineering, Waseda Univerity, 3-4-1 Ohkubo, Tokyo 169-8555, Japan

B11 Theoretical analysis of the electronic structure in valence band of H-terminated Si(111)
Y. Ogyu, T. Yamamoto and M. Uda, Department of Materials Science and Engineering, Waseda Univerity, 3-4-1 Okubo, Tokyo 169-8555, Japan

B12 Theoretical analysis of XPS spectrum of Al/Si interface
A. Hanta, K. Hirose*, T. Yamamoto and M.Uda, Department of Material Science and Engineering, Waseda University, *Institute of Space and Astronautical Science

13:50-14:50 "Keynote speech"

Chairperson: Yoshiyuki Kowada

B13 Application of DV-Xα calculations in ceramics science
Isao TANAKA, Department of Energy Science and Technology, Kyoto University

14:50-15:15 coffee break

15:15-15:50 "Materials Science Ⅱ"

Chairperson: Yoshiyuki Kowada

B14 Electronic State of Ca-doped $BaTiO_3$

Myung Chul Chang, Department of Materials Science and Engineering, Kunsan National University

B15 Raman Spectrum of Ca-doped $BaTiO_3$

Myung Chul Chang[*1)], Soo-Chang Yu[2)] [*1)]Department of Materials Science and Engineering, [2)]Department of Chemistry, Kunsan National University

B16 Theoretical Analysis of Bonding Interactions of the Nearest V-H Bonds in Vanadium Monohydride

Hiroyuki T. Takeshita[*1], Hirohiko Adachi [2], Hideaki Tanaka [1], Nobuhiro Kuriyama [1] and Itsuki Uehara,[1] Osaka National Research Institute, AIST, MITI,[2]Department of Materials Science and Engineering, Kyoto University

B17 Metal-metal bondings in p-block metal oxides

Motoki Sone[*], Hirohiko Adachi, Department of Material Science and Engineering, Kyoto University; Isao Tanaka, Department of Energy Science and Technology, Kyoto University; and Masataka Mizuno, Kobe Steel Corporation

B18 Chemical Bondings of Si segregated at grain boundaries in MgO ceramics

T. Mizoguchi[*], S. Nagano, F. Oba, M. Yoshiya, I. Tanaka, and H. Adachi, Department of Materials Science and Engineering, Kyoto University

15:50-16:10 "Relativistic effect"

Chairperson: Genta Sakane

B19 Relativistic Density-Functional Calculation for the Electronic Structure of Uranyl Nitrate

Masaru Hirata[*] and Turgut Bastug, Department of Materials Science, Japan Atomic Energy Research Institute (JAERI); Rika Sekine, Department of Chemistry, Faculty of Science, Shizuoka University; Jun Onoe, The Institute of Physical and Chemical Research (RIKEN); Hirohide Nakamatsu, Institute for Chemical Research, Kyoto University; and Shoichi Tachimori, Department of Materials Science, JAERI

B20 The Electronic Structure of Uranium Metal(3)

Masayoshi Kurihara, Nikkankyo; Masaru Hirata, JAERI; Rika Sekine, Shizuoka Univ.; Jun Onoe, RIKEN; and Hirohide Nakamatsu, Institute for Chemical Research, Kyoto Univ.

B21 Electronic Structure for Hydrated Lanthanide and Actinide Ions

Rika Sekine[*], Mai Shibukawa and Takahiro Hiroe, Dep. of Chemistry, Faculty of Sci., Shizuoka Univ.; and Masaru Hirata and Turgut Bastug, Dept. of Materials Science, JAERI

Comment

16:10-16:30 "Materials science by DV-X α Ⅲ"

Chairperson: Young Suk Kang

B22 Haldane Gap System: Electronic Structure and Magnetic Properties

T. Ishii[*], M. Kawahara, H. Hara, M. Kondo, H. Matsuzaka, and S. Kitagawa, Department of Chemistry, Tokyo Metropolitan University

B23 Electronic structures of $Li_{(1-x)}CoO_2$ (0<x<1)
Yukinori Koyama* and Isao Tanaka, Department of Energy Science and Technology, Kyoto University; and Hirohiko Adachi, Department of Materials Science and Engineering, Kyoto University

B24 Electronic Structure of Transparent Conductive $InGaZnO_4$ with an $YbFe_2O_4$ type Layered Structure
Masahiro Orita*[1], Masataka Mizuno[2], Isao Tanaka[3], Hirohiko Adachi[2]
[1]R&D Center, HOYA Corporation
[2]Department of Materials Science and Engineering, Kyoto University
[3]Department of Energy Science and Technology, Kyoto University

Comment

16:30 - 17:30 General meeting
17:30-18:30 Transportation(Hoam to Novotel Ambassdor)
18:30 - 21:00 Banquet

August 5

9:00-9:10 Official Comment

9:10-9:50 "Spectroscopy III"
Chairperson: Jun Yasui

C1 X-ray Emission Spectra of β-C_3N_4 Prepared by ECR Plasma Sputtering Method.
T. Kaneyoshi*, H. Kohzuki, M. Motoyama, and Hyogo Prefectural Institute of Industrial Research; Y. Tani, Y. Aoi, and E. Kamijyo, Ryukoku University; and Y. Muramatsu, NTT Integrated Information & Energy Systems Laboratories

C2 Theoretical analysis of Oxygen-K XANES spectra of Al_2O_3, Cr_2O_3 and Fe_2O_3
H. Kanno T.Yamamoto and M. Uda, Department of Materials Science and Engineering, Waseda Univerity, 3-4-1 Okubo, Tokyo 169-8555, Japan

C3 Theoretical analysis of O-K XANES spectra of Alkaline-earth Metal Oxides
A. Kanai, T.Yamamoto and M.Uda, Department of Materials Science and Engineering, Waseda Univerity, 3-4-1 Okubo, Tokyo 169-8555, Japan

C4 Theoretical analysis of O-K XANES spectra of MnO_2 and TiO_2
K. Akiyoshi, T.Yamamoto and M.Uda, Department of Materials Science and Engineering, Waseda University

C5 Theoretical XANES and Related Spectra
Hirohide Nakamatsu*, Song Bin, Kazuo Taniguchi, Rika Sekine, Takeshi Mukoyama, Hirohiko Adachi, Kyoto University, Osaka Electro-Communication University, Shizuoka University

C6 Analysis of O Kα EPMA Spectrum of Glassy State SiO_2–Na_2O Binary Slag

Masao Morishita* and Koichiro Koyama, Faculty of Engineering, Himeji Institute of Technology; Tadayoshi Kikko, Graduate Student of Himeji Institute of Technology; Masahiko Morinaga, Department of Materials Science and Engineering, Nagoya University; and Hirohiko Adachi, Department of Materials Science and Engineering, Kyoto University.

Comment

9:50–10:10 "Invited speech"

Chairperson: Masao Morishita

C7 Electronic States Calculations regarding the Role of Impurities on Ceramic Properties

Kimichika Fukushima* ,Power and Industrial Systems R&D Center, Toshiba Corporation

10:10–10:30 "Materials Science Ⅳ"

Chairperson: Hiroshi Yukawa

C8 Electronic Structures of Metal doped Bi_2Te_3 and Thermoelectricity

Sunao Sugihara, Seiji Kawashima, Hiroaki Suzuki, Shonan Institute of Technology; and R.Sekine*, Dept. of Chemistry, Faculty of Science Shizuoka University

C9 Chemical bonding of transition metal disilicides

Shigeto R. Nishitani*, Department of Materials Science and Engineering, Kyoto University, Kyoto 606-8501, Japan; Masataka Mizuno, Kobe Steel ltd., Takatsukadai 1-5-5, Nishi-ku, Kobe, 651-2271, Japan; Isao Tanaka, Department of Energy Science and Technology, Kyoto University,Kyoto, 606-8501, Japan; and Hirohiko Adachi, Department of Materials Science and Engineering, Kyoto University, Kyoto 606-8501, Japan

C10 The electronic structures of graphite, fullerene, and their compounds.

Shinji KAWASAKI*, Fujio OKINO and Hidekazu TOUHARA, Faculty of Textile Science & Technology, Shinshu University; Ning LIU and Toyohisa NAKAJIMA,
EPSON KOWA Corp.

10:30 - 11:00 coffee break

11:00–11:30 "Methodology"

Chairperson : Hirohide Nakamatsu

C11. Bond index and valency evaluation for DV-Xα

Katsumi Nakagawa* ,Canon Ecology Laboratory

C12 First-Principles Calculation of Multiplet Energy Including Electron Correlation Effects

Kazuyoshi Ogasawara*, Takugo Ishii and Hirohiko Adachi, Department of Materials Science and Engineering, Kyoto University; and Isao Tanaka, Department of Energy Science and Technology, Kyoto University

C13 Effect of Low Symmetry on Multiplet structures

Yukiko Ito*, Takugo Ishii, Kazuyoshi Ogasawara, and Hirohiko Adachi, Kyoto University

C14 First-Principles Calculation of Multiplet Structure in Chromium Ions Doped Laser Materials

Takugo Ishii*, Kazuyoshi Ogasawara, and Hirohiko Adachi, Department of Materials Science and Engineering, Kyoto University; and Isao Tanaka, Department of Energy Science and Technology, Kyoto University

11:30 Closing Ceremony

98年年会報告書

Reports of Korea-Japan DV-Xα Joint Symposium ('98)
<11th DV-Xα Annual Meeting>

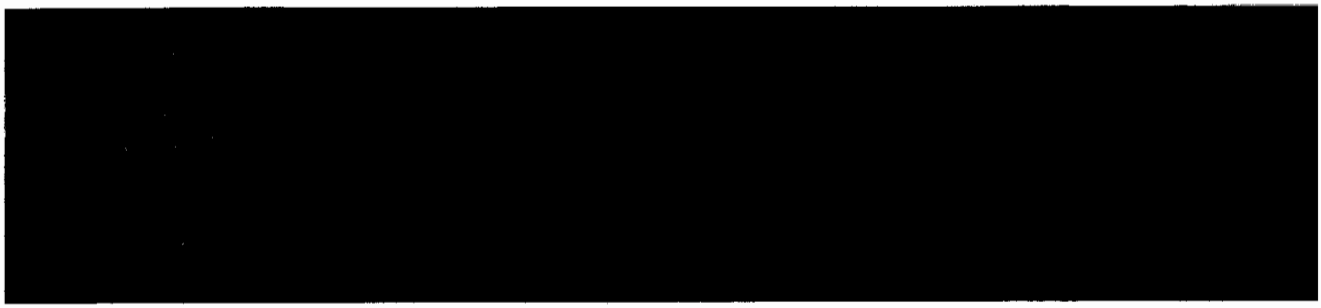
Index

DV-Xa研究協会会報, Vol. 11, No. 1 (1998)

1998年12月1日　発行

編集者　DV-Xα研究協会
発行人　DV-Xα研究協会
発行所　DV-Xα研究協会
〒531-0072　大阪市北区豊崎３丁目９番７号　いずみビル
（財）泉科学技術振興財団気付
振　替　01010-5-52330番　DVXA研究協会
印刷所　黒船印刷株式会社
〒422-8033　静岡市登呂二丁目４番２５号
電話　054-386-0236

Bulletin of the Society for Discrete Variational Xα
Vol. 11, No. 1 (1998)




DVXα