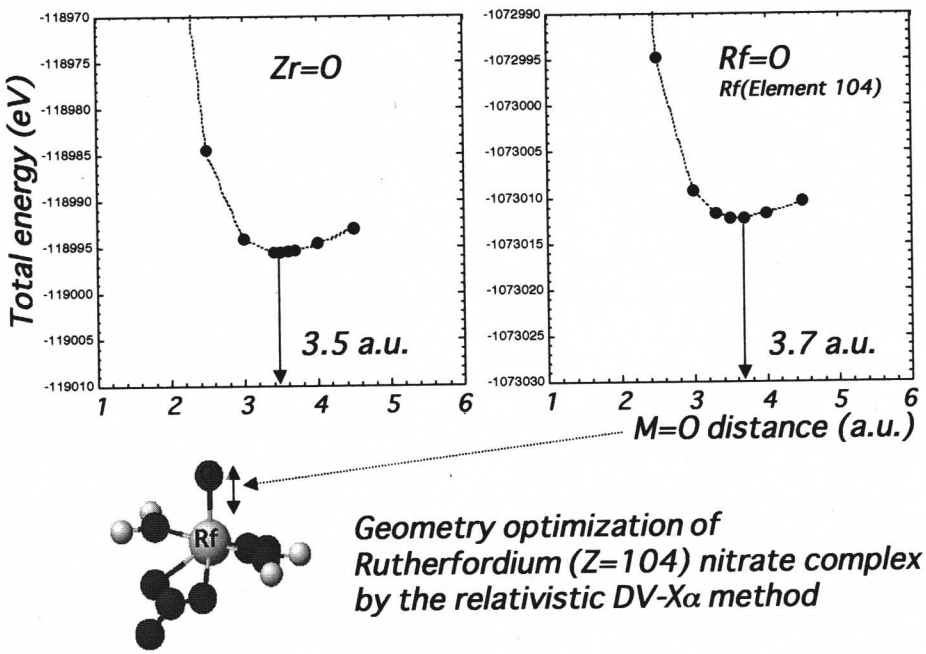
ISSN 1346−5015

DV-Xα 研究協会会報

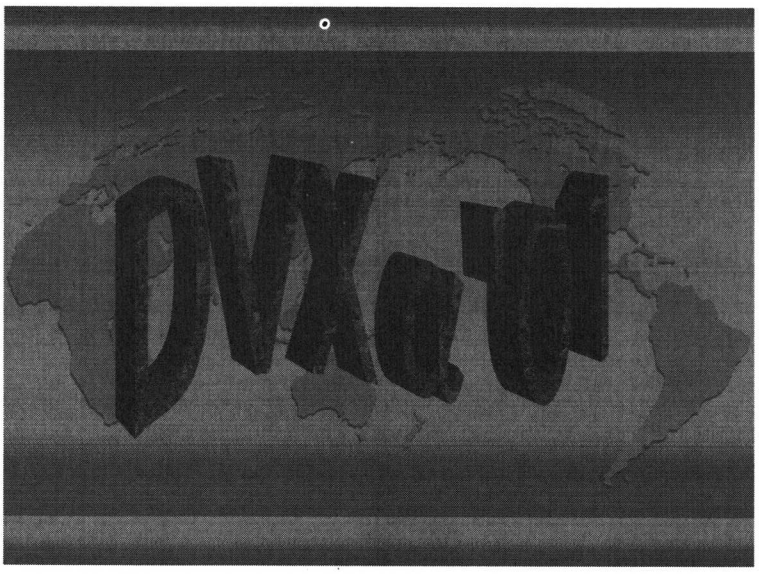
Bulletin of the Society for Discrete Variational Xα

Vol. 14, No. 1 (2001)



Geometry optimization of Rutherfordium (Z=104) nitrate complex by the relativistic DV-Xα method

編集　DV-Xα 研究協会



DVXα'01

DV-Xα International Workshop ('01)

&

14th Annual Meeting of the Society for DV-Xα Japan

(第 14 回 DV-Xα研究会)

July 31 - August 3, 2001

RIKEN, Saitama, Japan

The Society for Discrete Variational Xα

14th Annual Meeting of the Society for DV-Xα Japan （第 14 回 DV-Xα研究会）

会期：2001 年 7 月 31 日（火）～8 月 1 日（水）

会場：理化学研究所

生物科学研究棟　鈴木梅太郎ホール　（ポスタープレビュー）

1～4階ロビー　（ポスター会場）

大セミナー室Ｓ３１１　（運営・常任幹事　合同委員会）

〒351-0198　埼玉県和光市広沢 2-1

講演時間：一般講演　4 分（講演 2 分+質疑応答 2 分+ポスター掲示 4 日間）

DV-Xα International Workshop ('01)

August 1-3, 2001

RIKEN, 2-1 Hirosawa, Wako, Saitama 351-0198, Japan

Oral presentation	at Suzuki Umetaro Hall, Bioscience Building
Poster presentation	at Lobbies of the 1-4th floors, Bioscience Building
Getting Together	at Lobby of Suzuki Umetaro Hall, Bioscience Building
Banquet	at Welfare and Conference Building

Support of

Japan Society of Powder and Powder Metallurgy	(社) 粉体粉末冶金協会
The Ceramic Society of Japan	(社) 日本セラミックス協会
The Chemical Society of Japan	(社) 日本化学会
The Japan Institute of Metals	(社) 日本金属学会
The Japan Society for Analytical Chemistry	(社) 日本分析化学会
The Japan Society of Applied Physics	(社) 応用物理学会
The Japan Society of Mechanical Engineers	(社) 日本機械学会
The Mining and Materials Processing Institute of Japan	(社) 資源・素材学会
The Physical Society of Japan	(社) 日本物理学会
The Society of Materials Science, Japan	(社) 日本材料学会

Program-2

Program of the 14th Annual Meeting of the Society for DV-Xα

Japan （第 14 回 DV-Xα研究会）

7/31

12.50-13.00	Announcement from organizing committee	
13.00-13.10	M. Uda (Waseda Univ.)	Opening
13.10-13.20	H. Adachi (Kyoto Univ.)	Short Speech

Material Science (1)		
13.20-13.48	Chairperson: T. Yamamoto (RIKEN)	
Mater-01	R. Sekine (Shizuoka Univ.)	Density functional study on Zn metal clusters
Mater-02	S. Nagare (Keio Univ.)	Study on the band structure and impurity levels of ZnS:Mn phosphor
Mater-03	S. Itoh (Kyoto Univ. of Edu.)	Relativistic cluster calculation for rare earth doped GaAs
Mater-04	H. Nakatsugawa (Yokohama Nat. Univ.)	Electronic structure of $Sr_{1-x}La_xRuO_3$
Mater-05	K. Fukushima (Toshiba Co., IEC)	Electronic structure calculations for antiferromagentic and thermoelectric properties
Mater-06	K. Takai (Kwansei Gakuin Univ.)	Crystal structure of refractry metal silicides for ULSI applications
Mater-07	H. Yukawa (Nagoya Univ.)	Local electronic structures of hydrogen and phase stability of vanadium hydride, V_2H

Material Science (2)		
13.48-14.12	Chairperson: N. Ohashi (AML-NIMS)	
Mater-08	M. Hirata (JAERI)	Electronic structure of Am and Eu with N donor ligands
Mater-09	W. Takahara (Osaka Univ.)	Electronic structure and superconducting transition temperature of Laves phase V_2Zr compounds
Mater-10 (Canceled)		
Mater-11	S. Ono (Niigata Univ.)	Studies on origin of superionicity using band calculation and DV-Xα method
Mater-12	A. Kuwabara (Univ. of Tokyo)	Local bonding state and ionic conductivity in FSZ
Mater-13	M. Sasaki (Kyusyu Inst. of Tech.)	In_2O_3 based diluted magnetic semiconductor
Mater-14	M. Yoshino (Nagoya Univ.)	Protonic conductivity change with local electronic state around acceptor ions in perovskite-type oxide, $SrZrO_3$
14.12-14.32	Coffee Break	

Material Science (3)		
14.32-14.56	Chairperson: H. Yukawa (Nagoya Univ.)	
Mater-15	T. Miyamae (Kyoto Univ.)	Relativistic MO calculations with spin polarization on lanthanoid, actinoid compounds
Mater-16	W. Shin (AIST)	Electronic structure of $SrPbO_3$
Mater-17	T. Iitaka (RIKEN)	Order-N calculation of linear-response functions
Mater-18	T. Mukoyama (Kansai Gaidai Univ.)	Analytical wave functions for atoms by fitting numerical results with genetic algorithm
Mater-19	Y. Takahashi (AIST)	Structure and electron density study of the orthorhombic $LiMnO_2$ by X-ray structure analysis and first principle calculation
Mater-20	D. Lee (Korea Electrotechnology Res. Inst.)	Electronic Structure of IV-VI Compound Having Halite Structure, Calculated by DV- Xα Method

Surfaces, boundaries and Defects (1)		
14.56-15.24	Chairperson: K. Fukushima (Toshiba Co., IEC)	
Surf-01	Y. Sakai (Ashiya Univ.)	First-principles analysis of tunneling spectra for point defects on TiO_2 (110) surface
Surf-02	Y. Hayafuji (Kwansei Gakuin Univ.)	The electronic structures of defects in silicon clusters (1)
Surf-03	N. Esashi (Kwansei Gakuin Univ.)	The electronic structures of defects in silicon clusters (2)
Surf-04	H. Pinto (Nagoya Univ.)	Theoretical study of oxygen-vacancy defects in ferroelectric $BaTiO_3$
Surf-05	S. Yokota (Univ. of Tokyo)	Electronic structures of grain boundaries and high temperature deformation properties in oxide-doped 3Y-TZP
Surf-06	S. Sugihara (Shonan Inst. of Tech.)	Wetting property analysis of electrode metal and oxide ceramic at their interfaces using DV-Xα
Surf-07	K. Tanaka (Shizuoka Univ.)	Electronic study of ionic surface
15.24-15.44	Coffee Break	

Surfaces, boundaries and Defects (2)		
15.44-16.08	Chairperson: S. Sugihara (Shonan Inst. of Tech.)	
Surf-08	H. Moriwake (Matsushita Elec. Components Co., Ltd.)	First principles calculations of formation energy of Cr vacancy in $MgCr_2O_4$ spinel
Surf-09	T. Iitaka (RIKEN)	DFT-GGA Calculation of C_2H on Pd (110) surface
Surf-10	Y. Kim (AIST)	Li^+ extraction with $LiTm_{0.5}Mn_{1.5}O_4$ spinel in the aqueous phase (Tm = 3d transition metal)
Surf-11	T. Isobe (Shonan Inst. of Tech.)	Theoretical study on wetting properties of TiO_2 substrate with electrode metals
Surf-12	Y. Uchida (Hitachi, Co.,Ltd.)	The density of states of Cu with stacking faults
Surf-13	M. Matsui (Kyoto Univ.)	First principles calculation of charge compensative mechanism in oxides

Program-4

Organic and Inorganic Compounds		
16.08-16.36	Chairperson: Y. Kowada (Hyogo Univ. of Teacher Edu.)	
Org-01	J. Onoe (RIKEN)	Density-functional study on C_{60} photopolymerization
Org-02	Y. Liu (Nagoya Univ.)	Electronic state of lithium in carbonaceous materials
Org-03	T. Ishii (Tokyo Metro. Univ.)	Electronic structure and magnetic properties of metal porphyrins
Org-04	M. Fujiwara (Ryukoku Univ.)	Studies on molecular orbital calculations by the DV-Xα method and X-Ray photoelectron spectra of nickel(II) complexes.
Org-05	Y. Nakajima (Rikenkeiki Co.,Ltd.)	Near edge structure of porphyrin-complexes measured by PESA
Org-06	T. Segi (Osaka Univ.)	Isomer shift and quadrupole splitting of iron bis(N,N-dithiocarbamate)X complex (X = NO, Cl, Br, I)
Org-07	H. Yamashige (Fukuoka Univ.)	The electron structure of Fe, CoTPP complexes using the DV-Xα calculation
16.36-16.46	Announcement from organizing committee	

17.00-19.00	Poster Session
18.00-20.00	（運営・常任幹事）合同委員会（生物棟大セミナー室 S311）（委員のみ）

8/1

Spectroscopy (1)		
9.00-9.28	Chairperson: M. Mizuno (Osaka Univ.)	
Spec-01	Y. Iwata (Osaka Elec.-Commun. Univ.)	Studies of the electronic structure of lithium compounds by means of XPS and DV-Xα method
Spec-02	M. Nonaka (Kyushu Univ.)	Electronic structure of Mn-doped $ZnGa_2O_4$ using cluster calculation
Spec-03	J. Tsuji (Osaka Elec.-Commun. Univ.)	Studies of the Li-K XANES spectra of various lithium compounds
Spec-04	Y. Fukuda (Kyoto Univ.)	Analysis of Ni-L2,3 XANES in NiO by the first principles calculation
Spec-05	S. Matsuo (Fukuoka Univ.)	Al K-edge XANES spectral analyses of aqueous aluminum salt solutions by the DV-Xα calculation
Spec-06	D. Yamashita (Waseda Univ.)	L X-ray spectra emitted from 3d transition elements
Spec-07	M. Fujita (Shizuoka Univ.)	Assignment of Ti K-edge XANES spectra of $SrTiO_3$

Spectroscopy (2)		
9.28-9.52	Chairperson: Y. Muramatsu (JAERI)	
Spec-08	K. Fujimura (Kyoto Univ.)	Relativistic multiplet calculations of absorption spectra for rare-earth-based solid-state laser materials
Spec-09	K. Kuramoto (Himeji Inst. of Tech.)	Soft X-ray emission and absorption spectra in the O K reagion of aromatic compounds substituted with oxygenated functional groups
Spec-10	M. Yokomizo (Fukuoka Univ.)	DV-Xα XANES analysis for a Ni liquid metal complex
Spec-11	M. Kunisu (Kyoto Univ.)	ELNES/XANES of ZnO and AlN polytypes

Spec-12	J. Kawai (Kyoto Univ.)	Interpretation of the profile changes in fluorine K edge X-ray absorption spectra
Spec-13	A. Shigemi (Kyoto Univ.)	The dependence on geometry effect of Ni 2p XPS spectra

9.52-10.02	H. Wakita (Fukuoka Univ.)	Closing remarks

10.30-11.30	**General Meeting**

Program of the 3rd International Workshop on DV-Xα (DV-Xα'01)

8/1

13.25-13.30	Announcement from organizing committee	
13.30-13.35	M. Uda (Waseda Univ.)	Opening
	Present and Future Applications	
13.35-13.55 Invited-01	H. Adachi (Kyoto Univ.)	Brief reviews — Some progress of DV-Xα study —

Chairperson: M. Morinaga (Nagoya Univ.)		
13.55-14.25 Invited-02	D. E. Ellis (Northwestern Univ.)	Trying to uncover structure <=> functional relationships in complex systems
14.25-14.55 Invited-03	T. Sakuma (Univ. of Tokyo)	Localized quantum structure at ceramics grain boundary
14.55-15.25 Invited-04	K. Ogasawara, H. Adachi (Kyoto Univ.)	Relativistic discrete variational multi-electron (DV-ME) method
15.25-15.40	Coffee Break	

Atomic Spectroscopy		
Chairperson: J. Kawai (Kyoto Univ.)		
15.40-16.10 Invited-05	T. Mukoyama (Kansai Gaikokugo Univ.)	A new approach to electron transition during inner-shell ionization
16.10-16.40 Invited-06	L. Kover (ATOMKI, Hungary)	Interpreting Auger spectra in cluster approximation
16.40-17.00 Invited-07	Y. Muramatsu (JAERI)	Theoretically predicted soft X-ray emission spectra of graphitic-structured BC_2N
17.00-17.30 Invited-08	E. J. Nordgren (Uppsala Univ.)	Soft X-ray fluorescence and inelastic scattering studies of molecules and solids

17.45-18.00	Taking a Photo
18.00-20.00	Getting Together (Welcome party)

8/2 Morning

Materials Science		
Chairperson: T. Ishii (Tokyo Metro. Univ.)		
9.00-9.30 Invited-09	M. Sob, J. Kuriplach, H. Sorman (Inst. of Phys. of Mater., Acad. of Sci. of the Czech Republic)	Theoretical calculations of positron annihilation characteristics in inorganic solids — recent advances and problems
9.30-10.00 Invited-10	M. Mizuno (Osaka Univ.)	Theoretical calculation of positron lifetimes for defects in solids
10.00-10.30 Invited-11	M. Alatalo (Helsinki Univ. of Tech.)	Recent advances in the calculations for momentum distributions of annihilating electron-positron pairs in solids
10.30-10.50 Invited-12	Y. Koyama (Kyoto Univ.)	Factors determining intercalation voltages of lithium transition-metals oxides
10.50-11.05	Coffee Break	

Chairperson: R. Sekine (Shizuoka Univ.)		
11.05-11.35 Invited-13	H. Chang (Korea Res. Inst. of Chem. Tech.)	Electronic structure of chromium aluminum oxynitride
11.35-11.55 Invited-14	F. Oba, I. Tanaka, H. Adachi (Univ. of Tokyo)	Geometric and electronic structure of grain boundaries in ZnO
11.55-12.15 Invited-15	T. Nanba (Okayama Univ.)	XPS and DV-Xα studies on the electronic structure of silicate glasses
12.15-12.45 Invited-16	Y. Kowada (Hyogo Univ. of Teacher Edu.)	Electronic state of super-ionic conductors
12.45-13.05 Invited-17	N. Ohashi, T. Ikoma, H. Maki, H. Haneda, J. Tanaka (Adv. Mater. Lab., Nat. Inst. for Mater. Res.)	Quantum chemical approach to interfaces and surfaces of ceramics

13.10-17.45	(Lunch), Optional Tour

18.00-20.00	Banquet (Reception)

8/3 Morning

8.55-9.00	Announcement from organizing committee

Further Development		
Chairperson: M. Hirata (JAERI)		
9.00-9.30 Invited-18	M. Head-Gordon (U. C. Berkeley)	Fast methods for density functional theory calculation
9.30-9.50 Invited-19	T. Ishii (Kyoto Univ.)	Many-electron calculation for the analysis of the optical absorption spectra on impurity-metal center
9.50-10.20 Invited-20	P. Ordejon (Inst. de Ciencia de Barcelona)	First principles DFT calculations of electronic transport in molecular and nano-scale devices
10.20-10.40	Coffee Break	

Chairperson: J. Onoe (RIKEN)		
10.40-11.10 Invited-22	A. Nagy (Debrecen Univ.)	Excited states in the density functional theory
11.10-11.30 Invited-23	T. Yamamoto (RIKEN)	First principles calculations of lower-mantle minerals at high pressure
11.30-12.00 Invited-24	E. J. Brändas (Uppsala Univ., the editor of the Adv. Quantum Chem.)	Prorate spheroidal wavefunctions for signal processing

12.00	H. Wakita (Fukuoka Univ.)	Closing remarks

第 14 回 DV-Xα研究会報告書

Reports of 14th DV-Xα Annual Meeting

目次

※Ma: Mater, Su: Surf の略です。第一著者の名前のみしめしました。

※ 第 14 回 DV-Xα研究会のプログラムは 13-20 頁に掲載されています。

※ Surf-10 以後(Org-、Spec-)の講演番号の報告書は No.2 に掲載予定です。

＜編集後記＞ **今号の表紙は原子力研究所の平田　勝氏にお願いしました。**
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。編集者の不手際で関係の方々にご迷惑をおかけしたことをこの場をかりてお詫びいたします。

静岡大学　理学部化学科　関根理香
電子メール　scrseki@ipc.shizuoka.ac.jp

DV-Xα研究協会会報，Vol. 14, No. 1 (2001)

2001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. 14, No. 1 (2001)

ISSN 1346-5015