2012 年度スーパーコンピューティングシステム研究成果報告書
2012 年 4 月～2013 年 3 月

I. 研究内容概要

1. Adsorption Properties of Calix[*n*]arene n=4,6,8
   IMR, Tohoku University N.S. Venkataramanan, H. Mizuseki
   NICHe, Tohoku University Y. Kawazoe

2. 異種の微量元素を介在した Belite(β-C_2S)結晶の安定性とフォノン特性
   秋田工業高等専門学校 桜田良治
   Materials Research Centre, Indian Institute of Science Abhishek Kumar Singh
   東北大学 金属材料研究所 水関博志
   東北大学 未来科学技術共同研究センター 川添良幸

3. 金属ガラスの弾性域での繰り返し変形シミュレーション
   東北大学 原子分子材料科学高等研究機構 藤田武志, Yanhui Liu, 陳明偉

4. Catalytic Properties of Near-Surface Alloy of Transition Metal in Aluminum:
   A Density Functional Theory Study on Structural and Electronic Properties
   School of Physics and Technology, University of Jinan G. Chen
   IMR, Tohoku University H. Mizuseki
   NICHe, Tohoku University Y. Kawazoe

5. Ferromagnetism in Boron, Nitrogen and Carbon Substituted Yttria
   North Carolina State University Prithwish K. Nandi
   Bhabha Atomic Research Center Brahmananda Chakraborty
   NICHe, Tohoku University Yoshiyuki Kawazoe

6. New Cubic Carbon Phase Via Graphitic Sheet Rumpling
   Institute of Physics, Chinese Academy of Sciences Jian-Tao Wang
   Department of Physics, University of Nevada Changfeng Chen
   NICHe, Tohoku University Yoshiyuki Kawazoe

7. Tuning Magnetic Properties of Graphene Nanoribbons with Topological Line Defects
   Peking University Q. Sun, M. Kan, J. Zhou, Q. Wang
   NICHe, Tohoku University Y. Kawazoe
   Virginia Commonwealth University P. Jena

8. Patterning Graphitic C-N Sheets into Kagome Lattice for Magnetic Materials
   Peking University Q. Wang, X.W.Li, J. Zhou
   NICHe, Tohoku University Y. Kawazoe
   Virginia Commonwealth University P. Jena

9. Strain Induced Spin Crossover in Phthalocyanine-Based Organometallic Sheet
   Peking University J. Zhou, Q.Wang, Q. Sun
   NICHe, Tohoku University Y. Kawazoe
   Virginia Commonwealth University P. Jena

10. Theoretical Prediction of the Complexation Behaviors of Antitumor Platinum Drugs with Cucurbiturils
    Cauvery college of Engineering and Technology Suvitha Ambigapathy
    IMR, Tohoku University N.S.Venkataramanan, Hiroshi Mizuseki
    NICHe, Tohoku University Yoshiyuki Kawazoe

11. Influence of Exchange-Correlation Functional in the Calculations of Vertical Excitation Energies of Halogenated Copper Phthalocyanines using Time-Dependent Density Functional Theory (TD-DFT)
    Department of Chemistry, University of Ulsan Sang Uck Lee

12. Multi-scale Simulation of Nano-structured Devices from Electronic Structures to Mechanical Properties
    Graduate School of Engineering, Nagoya Institute of Technology Shuji Ogata

13. チタンクラスターによる窒素分子の解離
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14. DFT Study of Oxygen and Water Adsorption on Indium Oxide (111) Surface
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15. ビリアル定理に基づく高精度第一原理計算による多成分クーロン多体系の研究
横浜市立大学大学院 生命ナノシステム科学研究科 小山田隆行

16. Computational Study of the Fe-Si System from First-principles Calculations
Fracture and Reliability Research Institute, School of Engineering,
Tohoku University Arkapol Saengdeejing, Ying Chen, Ken Suzuki, Hideo Miura
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17. 鉄合金およびジルコニウム合金の照射損傷過程
- 格子間原子集合体の一次元運動過程のモデリング -
東北大学 金属材料研究所 佐藤裕樹, 阿部弘亨, 松永哲也

18. Study of FeSiBPCu Amorphous Structure by *Ab Initio* Simulation
IMR, Tohoku University Yaocen Wang, Masahiko Nishijima, Akihiro Makino
NICHe, Tohoku University Yoshiyuki Kawazoe

19. ナノ構造の電子状態から機械的性質までのマルチスケールシミュレーション
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20. 金属系構造材料の高性能化のためのマルチスケール組織設計・評価手法の開発
産業技術総合研究所 ユビキタスエネルギー研究部門 Vikas Sharma,
田中真悟, 香山正憲

21. 正二十面体準結晶におけるクラスタ配列
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22. Calculating the Curie Temperature of Magnetic Materials. Comparison of Three Different Approaches.
Corporate Sector Research and Advanced Engineering, Robert Bosch GmbH
Alberto Martinez-Limia, Adrien Gola, Lothar Kunz, Thomas Eckl
Research and Technology Center Asia Pacific, District Japan, Bosch Corporation
Takashi Shigematsu
IMR, Tohoku University Ryoji Sahara, Hiroshi Mizuseki
NICHe, Tohoku University Yoshiyuki Kawazoe

23. ナノ構造の電子状態から機械的性質までのマルチスケールシミュレーション
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24. Theoretical Investigation of Metal-Organic Frameworks (MOFs) & Organic Dyes for DSC
Faculty of Chemistry, University of Science, Vietnam National University
Nguyen-Nguyen Pham-Tran, Hung Q. Pham, Thi Nguyen
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Theory and Modeling Department, Culham Centre for Fusion Energy,
United Kingdom Atomic Energy Authority Duc Nguyen-Manh

25. Theoretical Study of Light Elements Dissolved in Bcc Iron
Japan Science and Technology Agency CREST
Maaouia Souissi, Hiroshi Numakura
Department of Materials Science, Graduate School of Engineering,
Osaka Prefecture University Maaouia Souissi, Hiroshi Numakura

26. 金属/酸化物/イオン液体界面の構造と電子状態の解明
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27. *Ab initio* Calculation of Graphene Nanodot Properties
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Visiting Scholar, Kenneth S. Pitzer Center for Theoretical Chemistry,
Chemistry Department, University of California Berkeley Michael R Philpott

28. A Theoretical Investigation on Adsorption Behavior of Ionic liquids on spinel MnO2(001) and Au(111) Electrode for Electrochemical Capacitor
WPI Advanced IMR, Tohoku University Sunho Jung, Kazuto Akagi

29. First-Principle Modeling of Graphene-Transition Metal Interactions
Faculty of Materials Science, University of Science Ho Chi Minh City
Hung M. Le, Viet Q. Bui
Theory and Modeling Department, Culham Centre for Fusion Energy,United Kingdom Atomic Energy Authority Duc Nguyen-Manh
NICHe, Tohoku University Yoshiyuki Kawazoe

30. First Principles Investigation on Functionalized Carbon Nanostructures for Different Applications

Department of Physics & Nanotechnology, SRM University K. Iyakutti
Department of Physics, Kongunadu College of Engg. and Tech V. J. Surya
School of Physics, Madurai Kamaraj University R. Lavanya, V. Vasu
IMR, Tohoku University H. Mizuseki
NICHe, Tohoku University Y. Kawazoe

31. 電池材料の第一原理シミュレーション

東北大学 金属材料研究所 池庄司民夫

32. First-principles study of formation of NdOx/Nd interface at Nd-Fe-B magnet

Institute of International Education & Department of Nanomechanics,
School of Engineering, Tohoku University Ying Chen

33. 全電子混合基底法プログラム TOMBO の整備

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34. Band Gap Engineering of Silicene Zigzag Nanoribbons with Perpendicular Electric Fields: a Theoretical Study

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35. Simultaneous Magnetic and Charge Doping of Topological Insulators with Carbon

Department of Physics, 2 Science drive 3, National University of Singapore
Lei Shen, Minggang Zeng, Yunhao Lu, Ming Yang, Yuan Ping Feng
School of Physics, Astronomy and Computational Science,
George Mason University Q.Y. Hu

36. Pressure-induced-amorphization of SiO_2 Revisited

WPI Advanced IMR, Tohoku University F. Takashi
School of Physics, Astronomy and Computational Science, George Mason University
H.W. Sheng

37. MCMC of Heisenberg-model with Reduced usage of FFT
IMR, Tohoku University Kazuhito Shida, Hiroshi Mizuseki
NICHe, Tohoku University Yoshiyuki Kawazoe

38. 2 次元フラストレート反強磁性体の厳密対角化法による研究
兵庫県立大学 物質理学研究科 中野博生

39. Effects of Doping of Au on the Atomic and Electronic Structure of Pd Nanoclusters
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40. 太陽電池用シリコン結晶における多結晶組織が応力分布に与える影響の解明
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徳本有紀, 米永一郎

41. 球形微粒子の自己組織化シミュレーション
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42. An Improved Lattice Boltzmann Model for Incompressible Flow
Department of Engineering Mechanics, Chongqing University
Z. Zeng, Liangqi Zhang, Haiqiong Xie
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NICHe, Tohoku University Y. Kawazoe

43. 強誘電体の電気熱量効果の直接的な分子動力学計算
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44. 高分子材料・金属材料にまたがる材料計算科学の基礎と連携
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手島正吾, 中村賢, 近藤恒, 荒木拓海
東京大学 大学院工学系研究科 物理工学専攻 伊藤伸泰, 青木尚登
東北大学 金属材料研究所 水関博志

45. 超伝導ナノ構造の転移温度上昇と磁束構造
大阪府立大学 工学研究科 加藤勝
秋田大学 教育文化学部 林正彦
東北大学 教養教育院 海老澤丕道
東北大学 金属材料研究所 小山富男, 西嵜照和
独立行政法人 物質・材料研究機構 超伝導物性ユニット 平田和人
東京大学 大学院工学系研究科 物理工学専攻 為ヶ井強
大阪府立大学工業高等専門学校 佐藤修
大阪府立大学 地域連携研究機構 川又修一
大阪府立大学 工学研究科 石田武和, 野口悟, 宍戸寛明, 丹羽祐平

46. 銅酸化物における複合励起状態の解明
日本原子力研究開発機構 先端基礎研究センター 森道康

47. 紫外・真空紫外透明ガラス材料の開発
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48. ミクロ-マクロ有限要素解析を用いた塑性加工問題の金属材料組織予測
独立行政法人 物質・材料研究機構 元素戦略材料センター 渡邊育夢

49. 熱電材料等の材料特性の計算機シミュレーションによる予測
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山口大学 メディア基盤センター 赤井光治

50. *Ab initio* Study on Electronic and Transport Properties of Topological Insulators in Nanoscale Sizes
IMR, Tohoku University Ahmad Ranjbar, Hiroshi Mizuseki
NICHe, Tohoku University Yoshiyuki Kawazoe

51. 第一原理計算を用いた新規な極性酸化物材料の探索と機能解析
名古屋工業大学 物質工学専攻 中山将伸

52. First-Principles Study on Crystal Structural Stability of Belite
Department of civil engineering at Akita National College of Technology
Ryoji Sakurada
NICHe, Tohoku University Yoshiyuki Kawazoe
Materials Research Centre, Indian Institute of Science Abhishek Kumar Singh

53. 全電子混合基底法プログラム TOMBO による新規水素貯蔵材料の開発
東北大学 金属材料研究所 佐原亮二, 水関博志
独立行政法人 物質・材料研究機構 構造材料ユニット 佐原亮二
デルフト工科大学 M. H. F. Sluiter
横浜国立大学 大学院工学研究院 大野かおる
東北大学 未来科学技術共同研究センター 川添良幸

54. 原子力関連材料の計算科学的研究
東北大学 金属材料研究所 小無健司, 八登唯夫, 三宅真紀
東京大学 大学院工学系研究科 原子力国際専攻 櫻原達也

55. Theoretical Study of Water Effect on Electronic Properties of Ionic Liquids
Nikolaev Institute of Inorganic Chemistry, SB RAS O.S. Subbotin, V. R. Belosludov
NICHe, Tohoku University O.S. Subbotin, V. R. Belosludov, Y. Kawazoe
IMR, Tohoku University R. V. Belosludov

56. Theoretical Study on Gas Storage in Clathrate Hydrates
IMR, Tohoku University R. V. Belosludov, H. Mizuseki
Nikolaev Institute of Inorganic Chemistry, SB RAS O.S. Subbotin, V. R. Belosludov
NICHe, Tohoku University Y. Kawazoe

57. The Van Der Waals Dispersion Coefficients within The All-Electron Mixed-Basis Tombo Approach
Nikolaev Institute of Inorganic Chemistry, SB RAS V. R. Belosludov, O. S. Subbotin
NICHe, Tohoku University V. R. Belosludov, O. S. Subbotin, Y. Kawazoe
IMR, Tohoku University R. V. Belosludov, H. Mizuseki

58. 新規医療用プローブ材料創製及び有効性計測と大規模計算との協同
独立行政法人 物質・材料研究機構 強磁場ステーション 根城均

59. 生体用コバルト合金の変形と結晶塑性有限要素解析
東北大学 金属材料研究所 小泉雄一郎, 松本洋明, 李云平, 黒須信吾, 千葉晶彦

60. 熱電材料等の材料特性の計算機シミュレーションによる予測
山口大学 メディア基盤センター 赤井光治
山口大学 大学院理工学研究科 仙田康浩, 嶋村修二

61. 放射光、中性子実験に向けた強磁場パルスマグネットの開発
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62. 液体シリコンプロセスに対する計算科学的研究
北陸先端科学技術大学院大学 情報科学研究科
今村光良, 本郷研太, 前園涼

63. 専用スーパーコンピューターを活用した統合マルチスケール材料設計による物理的、化学的性質解明
東北大学 金属材料研究所 水関博志

64. On the magnitude of zero-point vibration in one-component crystals
GREEN, National Institute for Materials Science Yong Yang
NICHe, Tohoku University, Yoshiyuki Kawazoe

65. 動的電子挙動を可能とする全電子混合基底第一原理計算プログラム開発とナノレベル新材料設計シミュレーション
東北大学未来科学技術共同研究センター　川添良幸

II. 原著論文

＜2012 年＞

1. Suzuki Segregation in Co–Ni-based Superalloy at 973 K: An Experimental and Computational Study by Phase-field Simulation
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and Yoshiyuki Kawazoe

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III. 国際会議発表論文

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2. Microscopic Investigation of Vortex-Vortex Interaction in Conventional Superconductors
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3. Quasi-Particle Structures Around a Pair of Half-Quantum Vortices in Chiral *p*-Wave Super Conductors
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5. Vortex States in Nano-Structured MgB_2
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   Shanghai, China(2011.10.27-29)
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   Shuji Shimamura, Takanori Takahira, Shota Suga, Hajime Tamura and Yasuhiro Senda

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   V. J. Surya, K. Iyakutti, H. Mizuseki and Y. Kawazoe

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   National Conference on Physics of New Materials(NCPNM-2012)
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   V. J. Surya, R. Lavanya, K. Iyakutti and Y. Kawazoe

2. First Principles Investigation on Hydrogen Storage in Single Walled Carbon Nanotubes Functionalized with Titanium Oxide
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   Noorul Islam University, Kumaracoil, Kanyakumari(2012.4.20-21)
   R. Lavanya, V. J. Surya, V. Vasu, K. Iyakutti and Y. Kawazoe

3. Charged Interfaces by First Principles Molecular Dynamics Simulations
   International Association of Colloid and Interface Scientists Conference(IACIS2012)
   Sendai International Center, Sendai, Japan(2012.5.13-18) No.S4B99 (Oral)
   T. Ikeshoji

4. Surface Morphology on Water Dissociation Coupled with Electron Transfer and OH Adsorption: First Principles Study
   11th ISE Spring Meeting
   Georgetown University, Washington, DC, USA(2012.5.23-25) No.56 (Oral)
   Y. Qian, I. Hamada, M. Otani and T. Ikeshoji

5. Solid Ionic Conductor and its Interface with Metal: First Principles Molecular Dynamics
   11th ISE Spring Meeting
   Georgetown University, Washington, DC, USA(2012.5.23-25) No.P-014 (Poster)
   Tamio Ikeshoji, Eiji Tsuchida, Tetsuya Morishita, Motoaki Matsuo,
   Yoshiyuki Kawazoe, and Shin-ichi Orimo

6. Proved Truth After 80 Years from Professor Slater's Misunderstanding by His Perturbation Theory
   The 16th International Annual Symposium on Computational Science and Engineering
   Chiang Mai University, Chiang Mai, Thailand (2012.5.23-25) (Invited)
   Y. Kawazoe

7. Interaction Between Interstitial and Substitutional Solute Atoms in Iron
   The 3rd International Symposium on Steel Science (ISSS 2012)
   Kansai Seminar House, Kyoto, Japan(2012.5.27-30) No.O03 (Oral)
   Numakura Hiroshi

8. First-principles Approach to the Nature of Light Elements Dissolved in α Iron
   The 3rd International Symposium on Steel Science (ISSS 2012)
   Kansai Seminar House, Kyoto, Japan(2012.5.27-30) No.P04 (Poster)
   Souissi Maaouia, Chen Ying and Numakura Hiroshi

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    Kansai Seminar House, Kyoto, Japan(2012.5.27-30)
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    Souissi Maaouia, Chen Ying and Numakura Hiroshi

11. First-principles study of thermodynamic and structural properties of Si-doped α-Fe
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    Kansai Seminar House, Kyoto, Japan(2012.5.27-30) No.P03 (Poster)
    A. Saengdeejing, Y. Chen, K. Suzuki, H. Miura and T. Mohri

12. Computational Approaches for Research and Design of Lithium Ion Battery Materials
    Accelrys Japan User Group Meeting
    Tokyo Conference Center, Tokyo, Japan (2012.6.1-2) (Invited)
    Sang Uck Lee

13. First-principles Calculation of Phase Equilibria and Phase Stability of Fe-Si System in Fe-rich Region
    CALPHAD 2012 Conference
    Berkeley, California, USA (2012.6.3-8) No.Tua7 (Oral)
    T. Mohri, Ying Chen and A. Saengdeejing

14. First Principles Investigation on Nanostructured Hydrogen Storage Materials
    14th International Congress of Quantum Chemistry(ICQC)
    University of Colorado Boulder, Boulder, Colorado, USA(2012.6.25-30)
    No.IV.30 (Poster)
    Hiroshi Mizuseki and Yoshiyuki Kawazoe

15. Atomistic Configuration in Fe-Si System in Fe- rich Region
    6th Korea-Japan Berkeley symposium on Advanced Materials
    Hearst Mining Building University of Calfornia, Berkeley, California, USA(2012.6.27-29) (Oral)
    T. Mohri, Y. Chen and A. Saengdeejing

16. Fast Li-ION Conductor: How the Ions Move in Solid Electrolyte $LiBH_4$
    The 13th Asian Conference on Solid State Ionics (ACSSI)
    Sakura Hall at Tohoku University, Sendai, Japan (2012.7.17-20)
    No.Oral-A8 (Oral)
    Tamio Ikeshoji, Eiji Tsuchida, Tetsuya Morishita, Kazutaka Ikeda, Motoaki Matsuo, Yoshiyuki Kawazoe and Shin-ichi Orimo

17. *Ab initio* Calculation to Predict Nanostructured Materials
    ACCMS - Theme Meeting on 2D Nanostructures : Graphene and Beyond
    Materials Research Center, Indian Institute of Science, Bangalore, India, (2012.7.29-30) (Plenary)
    Yoshiyuki Kawazoe

18. First-principles Investigation of Hydrogen Storage Properties in Nanostructured Storage Materials
    244th ACS National Meeting & Exposition
    Philadelphia, PA, U.S.A. (2012.8.19-23) No.495 (Invited)
    H. Mizuseki

19. Development of All-electron Mixed-basis *Ab Initio* Program TOMBO and Application for Developing Hydrogen Storage Materials
    244th ACS National Meeting & Exposition
    Philadelphia, PA, U.S.A. (2012.8.19-23) No.359
    Ryoji Sahara, Hiroshi Mizuseki, Marcel Sluiter, Kaoru Ohno
    and Yoshiyuki Kawazoe

20. Electrode and Electrolyte Interfaces and Reactions:
    First Principles Molecular Dynamics Study
    The 63rd Annual Meeting of the International Society of Electrochemistry
    Prague, Czech Republic (2012.8.19-24) (Oral)
    T. Ikeshoji

21. First-Principles Study on Structural Stability of Ba-DOPED Belite
    37th Conference on Our World in Concrete and Structures
    Singapole(2012.8.29-31) No.3B-7 (Oral)
    R. Sakurada, H. Mizuseki and A. K. Singh

22. First-principles Modeling of Formation of fcc-NdO_x at Nd/Nd-Fe-B Interface
    The 22nd International Workshop on Rare-Earth Permanent Magnets and
    Their Applications (REPM'12)
    NAGASAKI Brick Hall, Nagasaki, Japan(2012.9.2-5) No.O2-1700 (Oral)
    Ying Chen, Satoshi Hirosawa and Shiichi Iwata

23. Computational Approaches to Lithium Ion Battery Materials
    Korea Battery Society Korea(2012.9.19) (Invited)
    Sang Uck Lee

24. First principles Modeling of Formation and Stability of fcc-NdO_x at Nd/Nd-Fe-B Interface
    Discussion Meeting on Thermodynamics of Alloys (TOFA 2012)
    Pula, Croatia(2012.9.23-28) No.O11 (Oral)
    Y. Chen, S. Hirosawa and S. Iwata

25. Effect of Si to the Thermodynamic, Electronic, and Structural Properties of bcc-Fe: A Computational Study
    Materials Science and Technology 2012 Conference & Exhibition
    Pittsburgh, Pennsylvania, USA(2012.10.7-11) (Oral)
    A. Saengdeejing, Y. Chen, K. Suzuki, H. Miura and T. Mohri

26. Bias Imposed Interface Between Solid Li ion Conductor $LiBH_4$ and Li metal: First Principles Molecular Dynamics Simulations
    The Six Pacific Rim Meeting on Electrochemical and
    Solid-State Science (PRiME)
    Hawai`i Convention Center, Honolulu, USA (2012.10.7-12) (Oral)
    Tamio Ikeshoji, Eiji Tsuchida, Minoru Otani, Shigeyuki Takagi,
    Motoaki Matsuo, and Shin-ichi Orimo

27. Realization of Gas Storage Materials Based on Clathrate Hydrate: Computational Modelling
    Computational Modelling. Conference on Computational Physics (CCP2012)
    Nichii Gakkan Kobe Port Island Center, Kobe, Japan(2012.10.14-18)
    R. V. Belosludov, H. Mizuseki, O. S Subbotin, V. Belosludov
    and Y. Kawazoe

28. Atomic Force Microscopy Simulation by MD/continuum Coupling Method
    The 3rd Workshop on Computational and Statistical Physics (CSP3)
    Kyoto Research Park, Kyoto, Japan(2012.10.19-20) No.P-6 (Poster)
    Yasuhiro Senda, Nobuyuki Imahashi, Shuji Shimamura, Janne Blomqvist
    and Risto Nieminen

29. Effect of a Nickel cluster on the Dissociation Process of Hydrogen Molecule
    International Symposium on Metal-Hydrogen Systems 2012
    Kyoto TERRSA , Kyoto, Japan(2012.10.21-26) No.TuOC07 (Oral)
    Ryoji Sahara, Hiroshi Mizuseki, Marcel Sluiter, Kaoru Ohno
    and Yoshiyuki Kazwazoe

30. Theoretical Evaluation of Hydrogen Storage Capacity in Nanostructured Storage Materials
    International Symposium on Metal-Hydrogen Systems 2012
    Kyoto TERRSA , Kyoto, Japan(2012.10.21-26) No.ThOC08 (Oral)
    H. Mizuseki, R. Sahara, N. S. Venkataramanan, G. Chen and Y. Kawazoe

31. First-principles Study on Mechanical Properties of Dilute Si in Fe-Si Alloy
    2012 Fall Conference of the Korean Institute of Metals and Materials
    Changwon, Korea(2012.10.25-26) No.KJ-2 (Oral)
    Y. Chen, A. Saengdeejing, Ken Suzuki, Hideo Miura and T. Mohri

32. Charge Transfer Behavior at Organic Crystal Structures: OLED&OPV
    6th Accelrys Focused User Group Meeting (2012.11.17) (Invited)
    Sang Uck Lee

33. Study of Van Der Waals Dispersion Coefficients within the All-Electron Mixed-Basis Approach
    The Seventh General Meeting of Asian Consortium on Computational Materials Science - Virtual Organization (7th ACCMS-VO)
    Tohoku University, Sendai and Taikanso, Matsushima, Japan(2012.11.23-25) No.Inv-3 (Invited)
    V. R. Belosludov, O. S. Subbotin, V. V. Larin, R. V. Belosludov, H. Mizuseki and Y. Kawazoe

34. Simulation of Phase Composition and Formation Conditions of Methane and Carbon Dioxide Binary Hydrates.
    The Seventh General Meeting of Asian Consortium on Computational Materials Science - Virtual Organization (7th ACCMS-VO)
    Tohoku University, Sendai and Taikanso, Matsushima, Japan(2012.11.23-25) No.Inv-4 (Invited)
    O. S. Subbotin, T. P. Adamova, R. V. Belosludov, H. Mizuseki, Y. Kawazoe and V. R. Belosludov

35. First Principles Study of Hydrogen Storage in Bulk and Nano MgH_2
    The Seventh General Meeting of Asian Consortium on Computational Materials Science - Virtual Organization (7th ACCMS-VO)
    Tohoku University, Sendai and Taikanso, Matsushima, Japan(2012.11.23-25) No.Inv-6 (Invited)
    K. Iyakutti, Y. Kawazoe, R. Lavanya, V. J. Surya and V. Vasu

36. Charge Transfer Behaviors on the Organic Crystal Structures: OLED & OPV
    The Seventh General Meeting of Asian Consortium on Computational Materials Science - Virtual Organization (7th ACCMS-VO)
    Tohoku University, Sendai and Taikanso, Matsushima, Japan(2012.11.23-25)
    No.Inv-15 (Invited)
    Sang Uck Lee

37. Understanding the Role of Surface Step for Ti-Catalyzed Aluminum Hydrogenation
    The Seventh General Meeting of Asian Consortium on Computational Materials Science - Virtual Organization (7th ACCMS-VO)
    Tohoku University, Sendai and Taikanso, Matsushima, Japan(2012.11.23-25)
    No.Inv-20 (Invited)
    Gang Chen, Mengmeng Zheng, Shujuan Li, Yan Su, Hiroshi Mizuseki and Yoshiyuki Kawazoe

38. First Principles Study on Adsorption of Boron-Nitrogen Atoms in SWCNTs
    The Seventh General Meeting of Asian Consortium on Computational Materials Science - Virtual Organization (7th ACCMS-VO)
    Tohoku University, Sendai and Taikanso, Matsushima, Japan(2012.11.23-25)
    No.Oral-1 (Oral)
    V. J. Surya, K. Iyakutti, Y. Kawazoe, H. Mizuseki, R. Lavanya and V. Vasu

39. Charge Transfer Reaction at Solid-Liquid and Solid-Solid Interfaces by First Principles Molecular Dynamics Simulations
    The Seventh General Meeting of Asian Consortium on Computational Materials Science - Virtual Organization (7th ACCMS-VO)
    Tohoku University, Sendai and Taikanso, Matsushima, Japan(2012.11.23-25)
    No.Oral-2 (Oral)
    T. Ikeshoji

40. Introduction of TOMBO
    The Seventh General Meeting of Asian Consortium on Computational Materials Science - Virtual Organization (7th ACCMS-VO)
    Tohoku University, Sendai and Taikanso, Matsushima, Japan(2012.11.23-25)
    No.Oral-3 (Oral)
    R. Sahara

41. Structural Stability of Sr-Doped Belite
    The Seventh General Meeting of Asian Consortium on Computational Materials Science - Virtual Organization (7th ACCMS-VO)
    Tohoku University, Sendai and Taikanso, Matsushima, Japan(2012.11.23-25)
    No.Oral-17 (Oral)
    Ryoji Sakurada, Hiroshi Mizuseki, Yoshiyuki Kawazoe
    and Abhishek Kumar Singh

42. Roles of Oxygen Vacancies on Ferromagnetism in Ni Doped In_2O_3:
    A Hybrid Functional Study
    The Seventh General Meeting of Asian Consortium on Computational Materials Science - Virtual Organization (7th ACCMS-VO)
    Tohoku University, Sendai and Taikanso, Matsushima, Japan(2012.11.23-25)
    No.Oral-19 (Oral)
    Wei Wang, Hiroshi Mizuseki and Yoshiyuki Kawazoe

43. First Principles Study of the Effect of Magnetic and Non-Magnetic
    Dopants on the Opto-Electronic Properties of Indium Tin Oxide
    The Seventh General Meeting of Asian Consortium on Computational Materials Science - Virtual Organization (7th ACCMS-VO)
    Tohoku University, Sendai and Taikanso, Matsushima, Japan(2012.11.23-25)
    No.Oral-20 (Oral)
    Madhvendra Nath Tripathi, M. S. Bahramy, K. Shida, R. Sahara, H. Mizuseki
    and Y. Kawazoe

44. A Photon Intensity Correlation indicating Nonlinear Dynamics
    The Seventh General Meeting of Asian Consortium on Computational Materials Science - Virtual Organization (7th ACCMS-VO)
    Tohoku University, Sendai and Taikanso, Matsushima, Japan(2012.11.23-25)
    No.Oral-25 (Oral)
    H.Nejo, H.Mizuseki, Y.Kawazoe and A.Trifonov

45. Simulation of Structures and Phase Transitions for Helium Hydrates Based on Ice I_h and Ice II at Low Temperatures and High Pressures
    The Seventh General Meeting of Asian Consortium on Computational Materials Science - Virtual Organization (7th ACCMS-VO)
    Tohoku University, Sendai and Taikanso, Matsushima, Japan(2012.11.23-25)
    No.PS-2 (Poster)
    Yu. Yu. Bozhko, O.S. Subbotin, R. V. Belosludov, H. Mizuseki, Y. Kawazoe, V. R. Belosludov and V.M. Fomin

46. Theoretical Study of the Collective Vibration Features in Amorphous Ices
    The Seventh General Meeting of Asian Consortium on Computational Materials Science - Virtual Organization (7th ACCMS-VO)
    Tohoku University, Sendai and Taikanso, Matsushima, Japan(2012.11.23-25)
    No.PS-3 (Poster)
    K. V. Gets, O. S. Subbotin, V. R. Belosludov, R. V. Belosludov, H. Mizuseki and Y. Kawazoe

47. Thermodynamic Investigations of the Structures and Composition of Multicomponent Hydrates (N_2-O_2-CH_4-H_2O)
    The Seventh General Meeting of Asian Consortium on Computational Materials Science - Virtual Organization (7th ACCMS-VO)
    Tohoku University, Sendai and Taikanso, Matsushima, Japan(2012.11.23-25)
    No.PS-4 (Poster)
    T. P. Adamova, O. S. Subbotin, V. R. Belosludov, R. V. Belosludov, H. Mizuseki and Y. Kawazoe

48. H_2-Ar Clathrate Hydrates as a Hydrogen Storage Material
    The Seventh General Meeting of Asian Consortium on Computational Materials Science - Virtual Organization (7th ACCMS-VO)
    Tohoku University, Sendai and Taikanso, Matsushima, Japan(2012.11.23-25)
    No.PS-5 (Poster)
    Ravil Zhdanov, Oleg Subbotin, Vladimir Belosludov, Rodion Belosludov, Hiroshi Mizuseki and Yoshiyuki Kawazoe

49. *Ab inito* Study of Tuning Calixarenes for the Selective Sorption of Toxic Gases
The Seventh General Meeting of Asian Consortium on Computational Materials Science - Virtual Organization (7th ACCMS-VO)
Tohoku University, Sendai and Taikanso, Matsushima, Japan(2012.11.23-25)
No.PS-9 (Poster)
N.S. Venkataramanan, H. Mizuseki and Y. Kawazoe

50. Multicomponent Molecular Orbital Study on Positron Attachment to Atoms and Molecules Based on the Virial Theorem
The Seventh General Meeting of Asian Consortium on Computational Materials Science - Virtual Organization (7th ACCMS-VO)
Tohoku University, Sendai and Taikanso, Matsushima, Japan(2012.11.23-25)
No.PS-12 (Poster)
Takayuki Oyamada and Masanori Tachikawa

51. Light Elements Dissolved in α Iron: a First-principles Study
The Seventh General Meeting of Asian Consortium on Computational Materials Science - Virtual Organization (7th ACCMS-VO)
Tohoku University, Sendai and Taikanso, Matsushima, Japan(2012.11.23-25)
No.PS-18 (Poster)
Souissi Maaouia, Chen Ying and Numakura Hiroshi

52. First-principles Study of Phase Stability in Dilute Si-doped α-Fe
The Seventh General Meeting of Asian Consortium on Computational Materials Science - Virtual Organization (7th ACCMS-VO)
Tohoku University, Sendai and Taikanso, Matsushima, Japan(2012.11.23-25)
No.PS-19 (Poster)
Arkapol Saengdeejing, Ying Chen, Ken Suzuki, Hideo Miura and Tetsuo Mohri

53. On Smoothing of the Potential Landscape of the Ising Models with Random Coupling Constants
The Seventh General Meeting of Asian Consortium on Computational Materials Science - Virtual Organization (7th ACCMS-VO)
Tohoku University, Sendai and Taikanso, Matsushima, Japan(2012.11.23-25)
No.PS-21 (Poster)
K. Shida and Y. Kawazoe

54. Prediction and Analysis of the Cathode Catalyst Layer Performance of Proton Exchange Membrane Fuel Cells using Artificial Neural Network and Statistical Methods
    The Seventh General Meeting of Asian Consortium on Computational Materials Science - Virtual Organization (7th ACCMS-VO)
    Tohoku University, Sendai and Taikanso, Matsushima, Japan(2012.11.23-25)
    No.PS-27 (Poster)
    S. Ahadian, N. Khajeh-Hosseini-Dalasm, K. Fushinobu, K. Okazaki and Y. Kawazoe

55. The Study of Atomic Force Microscopy by Computer Simulation
    The Seventh General Meeting of Asian Consortium on Computational Materials Science - Virtual Organization (7th ACCMS-VO)
    Tohoku University, Sendai and Taikanso, Matsushima, Japan(2012.11.23-25)
    No.PS-34 (Poster)
    Nobuyuki Imahashi, Yasuhiro Senda, Shuji Shimamura, Janne Blomqvist and Risto Nieminem

56. Tersoff Potential Investigation on Grain Boundaries in Multicrystalline Silicon
    The Seventh General Meeting of Asian Consortium on Computational Materials Science - Virtual Organization (7th ACCMS-VO)
    Tohoku University, Sendai and Taikanso, Matsushima, Japan(2012.11.23-25)
    No.PS-36 (Poster)
    Hiroshi Mizuseki, Ryoji Sahara and Yoshiyuki Kawazoe

57. Micromagnetic Simulations on Hard and Soft Magnetic Granular Materials
    The Seventh General Meeting of Asian Consortium on Computational Materials Science - Virtual Organization (7th ACCMS-VO)
    Tohoku University, Sendai and Taikanso, Matsushima, Japan(2012.11.23-25)
    No.PS-37 (Poster)
    Hiroshi Mizuseki, Kazuhito Shida, Ryoji Sahara and Yoshiyuki Kawazoe

58. Atomistic Level Description of Ni Amorphous Solid
    The Seventh General Meeting of Asian Consortium on Computational Materials Science - Virtual Organization (7th ACCMS-VO)
    Tohoku University, Sendai and Taikanso, Matsushima, Japan(2012.11.23-25)
    No.PS-38 (Poster)
    R. V. Belosludov, D. V. Louzguine-Luzgin, A. Inoue, H. Mizuseki and Y. Kawazoe

59. Study of Electronic Structure and Thermoelectric Properties on Ba-Ga-Sn Clathrates
The Seventh General Meeting of Asian Consortium on Computational Materials Science - Virtual Organization (7th ACCMS-VO)
Tohoku University, Sendai and Taikanso, Matsushima, Japan(2012.11.23-25)
No.PS-39 (Poster)
K. Akai, Y. Kono, K. Kishimoto, S. Yamamoto and S. Shimamura

60. First principles calculation of the enhanced conductivity of MnO_2 by Au-doping
The Seventh General Meeting of Asian Consortium on Computational Materials Science - Virtual Organization (7th ACCMS-VO)
Tohoku University, Sendai and Taikanso, Matsushima, Japan(2012.11.23-25)
No.PS-40 (Poster)
L. J. Kang, J. L. Kang, M. W. Chen, H. Mizuseki and Y. Kawazoe

61. Theoretical and Computational Studies on Bi_2Se_3 as a Topological Insulator
The Seventh General Meeting of Asian Consortium on Computational Materials Science - Virtual Organization (7th ACCMS-VO)
Tohoku University, Sendai and Taikanso, Matsushima, Japan(2012.11.23-25)
No.PS-42 (Poster)
Ahmad Ranjbar, Hiroshi Mizuseki and Yoshiyuki Kawazoe

62. Theoretical Aspects of Gas Storage in Clathrate Hydrates for Realization Sustainable Future
2012 MRS Fall Meeting
Hynes Convention Center, Boston, MA, USA(2012.11.25-30)
No.G8.05 (Oral)
Rodion Belosludov, Oleg Subbotin, Hiroshi Mizuseki, Vladimir Belosludov and Yoshiyuki Kawazoe

63. Atomistic Level Description of Glass-transition Behavior of Zr-Cu-Al: Structural, Dynamic and Thermodynamic Properties
2012 MRS Fall Meeting
Hynes Convention Center, Boston, MA, USA(2012.11.25-30)
No.NN5.07 (Oral)
Rodion Belosludov, Yoshiko Yokoyama, Dmitrii Louzguine-Luzgin, Hiroshi Mizuseki, Yoshiyuki Kawazoe and Akihisa Inoue

64. Electronic Structures of Two-Dimensional Transition Metal Carbides and Nitrides: Mxenes
    2012 MRS Fall Meeting
    Hynes Convention Center, Boston, MA, USA(2012.11.25-30)
    No.B12.30 (Poster)
    Mohammad Khazaei, Masao Arai, Taizo Sasaki, Chan-Yeup Chung, Natarajan S. Venkataramanan, Mehdi Estili, Yoshio Sakka and Yoshiyuki Kawazoe

65. Computational Materials Science for Hydrogen Storage
    Summit of Materials Science (SMS2012)
    Tohoku University, Sendai, Japan(2012.11.27-30) No.S10 (Oral)
    H. Mizuseki

66. Molecular Level Description of Physical and Chemical Properties of Nanoporous Materials with Applications to Energy Storage
    2012 EMN Fall Meeting
    Red Rock Casino Resort and Spa, Las Vegas, Nevada, USA(2012.11.29-2)
    No.B31 (Invited)
    Rodion Belosludov

67. First Principles Study of Hydrogen Storage in SWCNT Functionalized with MgH_2
    The 57th DAE Solid State Physics Symposium 2012
    Indian Institute of Technology, Bombay, Mumbai, India(2012.12.3-7)
    AIP Conference Proceedings, **1512** (2012) pp.344-345 (Proceedings)
    R. Lavanya, K. Iyakutti, V. J. Surya, V. Vasu and Y. Kawazoe

68. Interaction of Carboplatin with SWCNT (10, 10): A First Principles Study
    The 57th DAE Solid State Physics Symposium 2012
    Indian Institute of Technology, Bombay, Mumbai, India(2012.12.3-7)
    AIP Conference Proceedings, **1512** (2012) pp.406-407 (Proceedings)
    V. J. Surya, K. Iyakutti, H. Mizuseki and Y. Kawazoe

69. Computational Approaches to Lithium Ion Battery Materials
    EHSRC Workshop 2012
    Korea(2012.12.13) (Invited)
    Sang Uck Lee

＜**2013** 年＞

1. Present Status of Computational Materials Science
   2013 ACCMS-WGM Asia Consortium on Computational Materials Science - Working Group Meeting on
   "Computational Design of Materials for Energy Conversion and Storage"
   National Taiwan University of Science and Technology, Taipei,
   Taiwan(2013.1.16-18) (Invited)
   Yoshiyuki Kawazoe

2. Introduction of TOMBO ～Development of Hydrogen Storage Materials～
   2013 ACCMS-WGM Asia Consortium on Computational Materials Science - Working Group Meeting on
   "Computational Design of Materials for Energy Conversion and Storage"
   National Taiwan University of Science and Technology, Taipei,
   Taiwan(2013.1.16-18) (Invited)
   Ryoji Sahara, Hiroshi Mizuseki, Marcel H. F. Sluiter, Kaoru Ohno
   and Yoshiyuki Kazwazoe

3. Theoretical Investigation of Graphene-M-Graphene (M=Cr,Fe) Intercalation Nanostructures Using Density Functional Approach
   2013 ACCMS-WGM Asia Consortium on Computational Materials Science - Working Group Meeting on
   "Computational Design of Materials for Energy Conversion and Storage"
   National Taiwan University of Science and Technology, Taipei,
   Taiwan(2013.1.16-18) (Invited)
   Hung M. Le. Yoshiyuki Kawazoe and Duc Nguyen-Manh

4. First-Principles Analysis of Hydrogen Storage Properties of Alkali-Doped Organic Materials
   2013 ACCMS-WGM Asia Consortium on Computational Materials Science - Working Group Meeting on
   "Computational Design of Materials for Energy Conversion and Storage"
   National Taiwan University of Science and Technology, Taipei,
   Taiwan(2013.1.16-18) (Invited)
   Hiroshi Mizuseki and Yoshiyuki Kawazoe

5. *Ab Initio* Design of Metal Catalysts and Compound Semiconductor Nanoparticles for Energy Applications
   2013 ACCMS-WGM Asia Consortium on Computational Materials Science - Working Group Meeting on
   "Computational Design of Materials for Energy Conversion and Storage"
   National Taiwan University of Science and Technology, Taipei,
   Taiwan(2013.1.16-18) (Invited)
   Vijay Kumar

6. Modulation of BN-C Hetero-Nanotubes by External Electric Fields : A First-Principles Study
   2013 ACCMS-WGM Asia Consortium on Computational Materials Science - Working Group Meeting on
   "Computational Design of Materials for Energy Conversion and Storage"
   National Taiwan University of Science and Technology, Taipei,
   Taiwan(2013.1.16-18) (Poster)
   Yunye Liang, Hiroshi Mizuseki and Yoshiyuki Kawazoe

7. First-Principles Study of Bi_2Se_3 as a Topological Insulator
   2013 ACCMS-WGM Asia Consortium on Computational Materials Science - Working Group Meeting on
   "Computational Design of Materials for Energy Conversion and Storage"
   National Taiwan University of Science and Technology, Taipei,
   Taiwan(2013.1.16-18) (Poster)
   Ahmad Ranjibar, Hiroshi Mizuseki and Yoshiyuki Kawazoe

8. Theoretical Prediction of Hydrogen Storage Materials for Sustainable Feature
   2013 ACCMS-WGM Asia Consortium on Computational Materials Science - Working Group Meeting on
   "Computational Design of Materials for Energy Conversion and Storage"
   National Taiwan University of Science and Technology, Taipei,
   Taiwan(2013.1.16-18) (Poster)
   N. S. Venkataramanan, H. Mizuseki and Y. Kawazoe

9. First-principles Study of Mechanical Properties of Fe-based Alloys
   The 1st Tsinghua Univ.-Tohoku Univ. Mini-Workshop in Tsinghua - International Workshop on Energy Materials and Reliability
   Tsinghua University, Beijing, China(2013.2.26-27)
   Ying Chen, A. Seangdeejing, K. Suzuki and H. Miura

10. A First Principles Study of Electronic and Elastic Properties in Borides
   MANA International Symposium 2013
   Epochal Tsukuba, Tsukuba, Japan (2013.2.27-3.1) No.PM-7 (Poster)
   R. Sahara, T. Shishido, A. Nomura, K. Kudou, S. Okada, V. Kumar and Y. Kawazoe

11. Theoretical Study of Gas Storage Materials Based on Clathrate Hydrate
   MANA International Symposium 2013
   Epochal Tsukuba, Tsukuba, Japan (2013.2.27-3.1) No.PP-3 (Poster)
   H. Mizuseki, R. V. Belosludov, O. S. Subbotin, V. R. Belosludov and Y. Kawazoe

12. An Improved MCMC of Heisenberg-model as an Example of Reduced usage of FFT
   MANA International Symposium 2013
   Epochal Tsukuba, Tsukuba, Japan (2013.2.27-3.1) No.PS-10 (Poster)
   Kazuhito Shida, Ryoji Sahara, Hiroshi Mizuseki and Yoshiyuki Kawazoe

13. Simulation Study of Gas Storage Materials Based on Clathrate Hydrates
   The 3rd AICS International Symposium
   RIKEN Advanced Institute for Computational Science, Kobe, Japan(2013.2.28-1) No.3P (Poster)
   H. Mizuseki, R. V. Belosludov, O. S. Subbotin, V. R. Belosludov and Y. Kawazoe

14. Mesoscopic Modeling on Granular Magnetic Media
   The 3rd AICS International Symposium
   RIKEN Advanced Institute for Computational Science, Kobe, Japan(2013.2.28-1) No.4P (Poster)
   H. Mizuseki, K. Shida, R. Sahara and Y. Kawazoe

15. Water Solubility Difference from the Natures of ($C_{20}H_{28}N_3O_3$) Br and ($C_{20}H_{28}N_3O_3$) NTf_2 Ionic Liquids.
    The 3rd AICS International Symposium
    RIKEN Advanced Institute for Computational Science, Kobe, Japan(2013.2.28-1) No.61P (Poster)
    O. Subbotin, R. Belosludov, R. Sahara, H. Mizuseki, V. Belosludov, Y. Kawazoe and T. Nakamura

16. Atomistic Level Description of Molecular/Atom Nano-structures Deposited on Si Surface
    Japan-Russia CVD Seminar
    Tohoku University, Sendai, Japan(2013.3.9) (Invited)
    R. V. Belosludov and H. Mizuseki

17. Atomistic Level Description of Phase Diagram of Gas Clathrate Hydrates with complex gas compositions
    2013 APS march meeting
    Baltimore, Maryland, USA(2013.3.18-22) No.C5.00004 (Oral)
    R. Belosludov, H. Mizuseki, Y. Kawazoe, O. Subbotin and V. Belosludov

18. *Ab-initio* Study of Structural and Electronic Properties of thin Film and Bulk Forms of Bi_2Q_3 (Q=Se, Te) as Topological Insulators
    2013 APS march meeting
    Baltimore, Maryland, USA(2013.3.18-22) No.V1.00321 (Poster)
    Ahmad Ranjbardizaj, Hiroshi Mizuseki and Yoshiyuki Kawazoe

IV. 紀要

＜2013 年＞

1. 文書管理システムの開発
    テクニカルセンター 技術研究報告, **25**(2013.3) pp.41-46
    一関京子, 五十嵐伸昭, 三浦重幸, 坂井泰雄, 勝倉真, 八鍬友一

2. 材料設計専用スーパーコンピューティングシステム
テクニカルセンター 技術研究報告, **25**(2013.3) pp.47-53
五十嵐伸昭, 一関京子, 佐藤和弘, 野手竜之介, 三浦重幸, 石川真二,
八鍬友一, 勝倉真, 松本秀一, 三森悟毅, 水関博志, 川添良幸

3. スーパーコンピューティングシステムにおける
ストレージシステム利用状況表示システムの開発
テクニカルセンター 技術研究報告, **25**(2013.3) pp.55-60
五十嵐伸昭, 一関京子, 石川真二, 八鍬友一, 勝倉真

V. 予稿集

＜2011 年＞

1. 合金における格子間原子集合体と溶質原子の相互作用モデル
日本金属学会 2011 秋期 第 149 大会
沖縄コンベンションセンター(2011.11.7-9) No.205 (Poster)
佐藤裕樹, 阿部弘亨, 金思雄, 松永哲也

＜2012 年＞

1. Fe-Si 二元合金における Si 希薄領域の不規則相の局所原子配列の
第一原理計算
日本金属学会 2012 春期 第 150 大会
横浜国立大学 常盤台キャンパス(2012.3.28-30) No.111 (Oral)
毛利哲雄, 陳迎

2. 新スーパーコンピューティングシステムの概要
第 123 回 東北大学金属材料研究所講演会 (2012 年春季)
東北大学 金属材料研究所(2012.5.23-24) No.37 (Poster)
五十嵐伸昭, 一関京子, 野手竜之介, 三浦重幸, 佐藤和弘, 八鍬友一,
勝倉真, 松本秀一, 石川真二, 三森悟毅, 水関博志, 川添良幸

3. Adsorption of Ammonia Over CNT- a Mechanistic Study using *Ab Inito* Study.
ナノ学会第 10 回大会
大阪大学(2012.6.14-16) No.O-16 (Oral)
Abhijit Chatterjee, R. Venkataraman and Yoshiyuki Kawazoe

4. A Nanometer-Scale Spectroscopy using Near-Filed Detection Through Nano-Holes
   ナノ学会第 10 回大会
   大阪大学(2012.6.14-16) No.O-22 (Oral)
   根城均, 水関博志, 川添良幸

5. The Silicene Sheet and Silicene Nano Ribbons under the Electric Fields: A First-Principles Study
   ナノ学会第 10 回大会
   大阪大学(2012.6.14-16) No.P1-28 (Poster)
   Y. Liang, H. Mizuseki and Y. Kawazoe

6. *Ab initio* Calculation of Anticancer Drugs Encapsulated for Drug-Delivery
   ナノ学会第 10 回大会
   大阪大学(2012.6.14-16) No.P2-21 (Poster)
   N. S. Venkataramanan, 根城均, 水関博志, 川添良幸, 権田幸祐, 多田寛, 大内憲明

7. First-Principles Study on New Hydrogen Storage Nanomaterials
   ナノ学会第 10 回大会
   大阪大学(2012.6.14-16) No.P2-61 (Poster)
   水関博志, 佐原亮二, V. Wang, N. S. Venkataramanan, G. Chen, 川添良幸

8. An Extended Version of Bootstrap Percolation Model.
   ナノ学会第 10 回大会
   大阪大学(2012.6.14-16) No.P2-63 (Poster)
   志田和人, 佐原亮二, 水関博志, 川添良幸

9. Theoretical Study of Electronic and Transport Properties of Atomic Nanowires Deposited on Silicon Surface
   ナノ学会第 10 回大会
   大阪大学(2012.6.14-16) No.P2-65 (Poster)
   R. V. Belosludov, A. A. Farajian, H. Mizuseki, K. Miki and Y. Kawazoe

10. Development of All-Electron Mixed-Basis *Ab Initio* Program TOMBO and Application for Developing Hydrogen Storage Materials
    ナノ学会第 10 回大会
    大阪大学(2012.6.14-16) No.P2-66 (Poster)
    佐原亮二, 水関博志, Marcel Sluiter, 大野かおる, 川添良幸

11. 原子モデルを用いたシリコン結晶粒界評価
太陽電池材料開発の現在と未来　-第 5 回半導体若手ワークショップ-
東北大学 金属材料研究所(2012.7.30-2012.7.31) No.15 (Oral)
水関博志, A. Suvitha, 佐原亮二, 川添良幸

12. Theoretical Investigation of Grain Boundaries in Multicrystalline Silicon
太陽電池材料開発の現在と未来　-第 5 回半導体若手ワークショップ-
東北大学 金属材料研究所(2012.7.30-2012.7.31) No.76 (Poster)
Hiroshi Mizuseki, Ambigapathy Suvitha, Ryoji Sahara
and Yoshiyuki Kawazoe

13. ビリアル定理に基づいた多成分系分子軌道法による陽電子化合物の研究
分子研研究会 - レーザー分光および磁気測定による分子構造探求の新展開
分子科学研究所, 愛知(2012.7.30-31) (Oral)
小山田隆行, 立川仁典

14. Light elements dissolved in α iron: A Density Functional Theory study
日本金属学会 2012 秋期 第 151 大会
愛媛大学 城北キャンパス(2012.9.17-19) No.465 (Oral)
Souissi Maaouia, Chen Ying and Numakura Hiroshi

15. ビリアル定理を満たす多成分分子軌道法による陽電子化合物の研究
第 6 回分子科学討論会
東京大学 本郷キャンパス(2012.9.18-21) No.1P-093 (Poster)
小山田隆行, 立川仁典

16. 鉄中の軽元素– 第一原理計算による研究
合金状態図 第 172 委員会 第 24 回委員会･研究会
物質材料研究機構, 筑波(2012.10.29-30) (Oral)
Souissi Maaouia, Chen Ying and Numakura Hiroshi

17. First-principles Calculation of the Mechanical Properties of Dilute Si in Fe-Si Alloy
合金状態図 第 172 委員会 第 24 回委員会･研究会
物質材料研究機構, 筑波(2012.10.29-30) (Proceed)
Ying CHEN, Arkapol SAENGDEEJING and Tetsuo MOHRI

18. First Principles Calculations of Positive Electrode Materials in Ni-MH Battery
第 53 回電池検討会
ヒルトン福岡シーホーク, 福岡(2012.11.14-16) No.3E24 (Oral)
池庄司民夫, 大谷実, 森下徹也, 信原邦啓

19. Impact of Surface Morphology on the Reaction Dynamics of Pt/water Interface
第 53 回電池検討会
ヒルトン福岡シーホーク, 福岡(2012.11.14-16) (Oral)
Y. Qian, Y. Zhao, M. Otani, T. Ikeshoji

20. 全電子混合基底法プログラム TOMBO による水素貯蔵材料の開発
第 11 回 日本金属学会東北支部大会
東北大学 片平さくらホール(2012.12.13) No.P-2 (Poster)
佐原亮二, 水関博志, Marcel Sluiter, 大野かおる

＜2013 年＞

1. オーダーN 実空間 DFT 法を用いたハイブリッド量子古典シミュレーション
スーパーコンピュータワークショップ 2013
自然科学研究機構 岡崎コンファレンスセンター(2013.1.22-23) (Invited)
尾形修司

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