

2019年度スーパーコンピューティングシステム

利用研究成果報告書

(2019年4月～2020年3月)

目 次

『巻頭言』……………計算材料学センター長 久保百司

I. 研究内容概要

1. ホウ素錯体を電子アクセプタとする高性能n型半導体の開発1
名古屋工業大学大学院工学研究科 小野克彦
2. エーライト(C₃S)への水分子吸着機構の数値解析.....4
秋田工業高等専門学校 桜田良治
東北大学金属材料研究所 Rodion Vladimirovich Belosludov
日本大学 鵜澤正美
太平洋セメント(株) 細川佳史
東北大学未来科学技術共同研究センター 川添良幸
Materials Research Centre, Indian Institute of Science, India
Abhishek Kumar Singh
3. 固溶型合金ナノ粒子触媒の分子吸着特性6
物質・材料研究機構 古山通久、難波優輔

4. ノンコリニア非磁性体の系統的第一原理計算 8
東京大学新領域創成科学研究科、理化学研究所創発物性科学研究センター
Marie-Therese Huebsch
東北大学金属材料研究所 鈴木通人
東京大学大学院工学系研究科 有田亮太郎
5. 第一原理分子動力学法による固体酸化物触媒の機能解明 10
東京大学大学院工学系研究科化学システム工学専攻 中山哲
6. 点欠陥の照射誘起移動過程の分子動力学計算 13
広島工業大学 佐藤裕樹
7. 有限要素法を用いたタンクステン材料の熱・応力構造解析 16
九州大学応用力学研究所 徳永和俊
九州大学総合理工学府 堀田智宏、浮田天志、尾崎浩詔
8. 第一原理計算および量子多体計算に基づく多バンド系の超伝導機構 18
新潟大学理学部 大野義章
新潟大学自然科学研究科 関川卓也、齋藤雅樹、小林健太郎
9. 固体中のイオン伝導の分子動力学シミュレーション 21
産業技術総合研究所数理先端材料モデリングオープンイノベーションラボ
ラトリ 中西毅、池庄司民夫、Sau Kartik
東北大学金属材料研究所水素機能材料工学研究部門 高木成幸
10. クラスター複合物質の化学的性質解明へ向けた実験および理論的研究 26
豊田工業大学 市橋正彦、安松久登
九州大学大学院理学研究科 寺寄亨
東北大学金属材料研究所 Rodion Vladimirovich Belosludov
11. 第一原理計算による有機修飾金属酸化物ナノ粒子の構造物性の解明 28
名古屋大学大学院工学研究科 高見誠一
東北大学材料科学高等研究所 横哲
12. 磁歪効果を含めた高性能磁性材料の設計と大規模シミュレーション手法開発 32
高エネルギー加速器研究機構物質構造科学研究所 塚原宙、小野寛太

13. 有機π共役ドナー・アクセプター材料物性の理論研究 37
日本女子大学理学部数物科学科 村岡梓、太田希、阿部文香、池山すみれ、
寿崎文音、畠中ひなこ
14. イオン伝導機構を用いた新規メモリデバイス開発に向けた第一原理計算 40
東京大学工学系研究科マテリアル工学専攻 清水康司、渡邊聰
15. リチウムイオン二次電池用電極材料の結晶粒子形状制御解析 43
信州大学先鋭材料研究所 椎葉寛将、原健治郎、是津信行、手嶋勝弥
16. 金属表面上の磁性分子のスピノン状態に関する第一原理計算 46
分子科学研究所 南谷英美
17. 鉛フリー有機無機ペロブスカイトの電子状態計算 49
九州工業大学 飯久保智、井手敦子
18. Phase transformation assisted twinning in a face-centered-cubic FeCrNiCoAl_{0.36} high-entropy alloy 52
City University of Hong Kong, Osaka University Peijun Yu
The University of Tennessee Rui Feng, Bilin Chen, Peter K. Liaw
Osaka University, Kyoto University Junping Du, Shigenobu Ogata
Osaka University Shuhei Shinzato
City University of Hong Kong Jyh-Pin Chou
National Chiao Tung University Yu-Chieh Lo
City University of Hong Kong, Department of Materials Science and Engineering,
City University of Hong Kong, City University of Hong Kong Shenzhen Research
Institute Alice Hu
19. 有機導体・半導体の電子構造解析 56
東北大学大学院理学研究科 瀧宮和男、川畑公輔
20. 燃料電池電解質材料におけるフォノン解析と水和構造の最適化 61
東北大学大学院理学研究科物理学専攻 松井広志、高野紗季
21. 完璧なπ共役二次元シートを持つフラットシリセンの設計 65
東北大学大学院農学研究科 高橋まさえ

22. Interaction and diffusion of atomic oxygen in monovacancy-containing Cr-and Ti-doped nickel structures 67
New Industry Creation Hatchery Center, Tohoku University, Japan
Nishith K. Das and T. Shoji
23. フォノンバンドエンジニアリングによる Fe 系熱電変換材料の高性能化 72
東北大学金属材料研究所 岡本範彦、藤原浩輔、市坪哲
24. 反強磁性体の異常ホール効果と電子構造トポロジーの研究 74
東北大学金属材料研究所 鈴木通人、Vu Thi Ngoc Huyen、柳有起
25. 金属積層造形プロセスにおける溶融凝固挙動の解析 77
東北大学金属材料研究所 青柳健大
26. 高水素配位錯イオンの擬回転を利用した室温超イオン伝導 82
東北大学金属材料研究所 高木成幸、横山凱乙、遠藤亘
東北大学材料高等研究所 池庄司民夫
27. 籠状クラスター型錯イオンを有するクロソ系錯体水素化物におけるイオン伝導機構の解明 85
東北大学金属材料研究所 金相侖、高木成幸
28. Interatomic interactions in Co–Ni–Cr–Mo alloys 87
Institute for Materials Research, Tohoku University J. Li, K. Yamanaka and
A. Chiba
29. 大規模第一原理計算による耐熱材料の相安定性と電子状態解析 92
物質・材料研究機構 佐原亮二、S. K. Bhattacharya、M. Souissi、大塚秀幸
韓国科学技術研究院 水閥博志、Ram Babu
Indian Institute of Science Education and Research (IISER) Prasenjit Ghosh,
Kanika Kohli
30. 高信頼性第一原理シミュレーション計算によるマテリアルインフォマティクスを用いた新単結晶材料探索 94
東北大学未来科学技術共同研究センター 横田有為

31. 新規籠型構造及び二次元構造ナノ材料設計 99
東北大学大学院医工学研究科 松木英敏
32. High accuracy first-principles calculation of thermodynamic and diffusion properties 103
School of Engineering, Tohoku University Ying Chen, Arkapol Saengdeejing,
Nguyen-Dung Tran, Theresa Davey, Qinqiang Zhang, Mariko Kadowaki
School of Materials Science and Engineering Shanghai University Hao Wang
Beijing University of Science and Technology Lei Wang
Institute of Fluid Physics Hua Y. Gneg
Institute of Physics, Slovak Academy of Sciences Ivan Štich, Jan Brndiar
NIMTE, Chinese Academy of Sciences Hubin Luo
Indian Institute of Science Education and Research (IISER) Kabir Mukul
33. 磁歪発電素子開発を目的とした新材料設計のための第一原理計算 108
東北大学金属材料研究所 梅津理恵
34. 大規模分子動力学シミュレーションによるマルチスケール現象の解明と新規材料設計への応用 111
東北大学金属材料研究所 尾澤伸樹、大谷優介、宮崎成正、許競翔、王楊、
陳茜、上原周一、木村颯太、柳澤穂波、山下周郎、久保百司
35. ROLE OF NON-COVALENT INTERACTION IN DESCRIPTION OF THE ELECTRONIC, DYNAMIC AND THERMODYNAMIC PROPERTIES OF NANOPOROUS MATERIALS FOR ECO-FRIENDLY ENERGY APPLICATIONS 115
Institute for Material Research, Tohoku University R. V. Belosludov
36. 分子と結晶の両方の全電子スペクトル計算プログラムの開発 120
横浜国立大学大学院工学研究院 大野かおる、Mohamad Khazaei
マレーシア・マラヤ大学 Khian-Hooi Chew
東北大学金属材料研究所 Rodion Belosludov

37. マルチスケール計算による多元材料の材料物性と相の安定性の研究とその理工系高等教育への適用 122
東北大学金属材料研究所計算物質科学人材育成コンソーシアム 寺田弥生
ICMPE France Jean-Claude Crivello
Korea Institute of Materials Science, Korea Eun-Ae Choi
Universidade Federal Fluminense Brazil Paulo Rios, Assis Weslley,
Ventura Harison
熊本大学大学院自然科学研究科 連川貞弘、上村宗二朗
東北大学大学院工学研究科 吉見享祐
38. イオン液体の電気化学特性の分子シミュレーションによる研究 127
東京大学情報基盤センター 芝隼人
東北大学金属材料研究所 ボノー パトリック
39. Theoretical design toward abundant element nanocatalysts 132
Faculty of Science & WPI-ICReDD, Hokkaido University Andrey Lyalin,
Sonu Kumar, Takeshi Iwasa and Tetsuya Taketsugu
40. マルチスケール流動シミュレーション用プラットフォームの開発 135
東北大学大学院理学研究科 村島隆浩、森井洋平、川勝年洋
41. 高信頼性構造材料（ポスト「京」重点課題(7)サブ課題E） 138
産業技術総合研究所電池技術研究部門 香山正憲、徐卓、田中真悟
産業技術総合研究所機能材料コンピュテーションナルデザイン研究センター
石橋章司
名古屋工業大学 田村友幸
横浜国立大学大学院工学研究院 大野かおる、Thi Nu Pham
物質・材料研究機構 佐原亮二
42. Atomistic Simulations of Carbon Diffusion in BCC Iron with Point Defect 145
Institute for NanoScience Design, Osaka University Tien Quang Nguyen
Graduate School of Engineering, Osaka University Kazunori Sato, Yoji Shibutani
43. 軽元素B,C,N系積層原子膜の物性解明と電子デバイス材料への応用 149
東京工業大学理学院 斎藤晋、藤本義隆、伊藤智哉

II. 原著論文

<2019年>

1. Adsorption of water on fluorinated graphene 153
J. Phys. Chem. Solids, 124 (2019) pp.54-59
Yong Yang, Fuchi Liu and Yoshiyuki Kawazoe
2. Subatomic-scale resolution with SPM: Co adatom on $p(2 \times 1)$ Cu(110):O 159
Nanotechnology, 30 (2019) Art.No.095703
R Turanský, K Palotás, J Brndiar, Y J Li, Y Sugawara and I Štich
3. Thermal transport properties of penta-graphene with grain boundaries 166
Carbon, 145 (2019) pp.445-451
Jie Sun, Yaguang Guo, Qian Wang and Yoshiyuki Kawazoe
4. Many-Body Quantum Monte Carlo Study of 2D Materials: Cohesion and Band Gap in Single-Layer Phosphorene 173
Phys. Rev. X, 9 (2019) Art.No.011018
T. Frank, R. Derian, K. Tokár, L. Mitas, J. Fabian and I. Štich
5. Interfacial properties of penta-graphene-metal contacts 181
J. Appl. Phys., 125 (2019) Art.No.065308
Arzoo Hassan, Yaguang Guo, Qian Wang, Yoshiyuki Kawazoe and Puru Jena
6. Phase diagram and composition of water based crystalline phases in hydrogen – Water binary system 188
Solid State Commun., 294 (2019) pp.6-10
Ravil K. Zhdanov, Yulia Y. Bozhko, Vladimir R. Belosludov, Oleg S. Subbotin, Kirill V. Gets, Rodion V. Belosludov and Yoshiyuki Kawazoe
7. N-doped peanut-shaped carbon nanotubes for efficient CO₂ electrocatalytic reduction 193
Carbon, 152 (2019) pp.241-246
Wenyang Zhou, Haoming Shen, Qian Wang, Jun Onoe, Yoshiyuki Kawazoe and Puru Jena

8. Phase Stabilities of Stable β - and Metastable β' - Cu₄Ti Intermetallic Compounds in The Cu-Ti-Ni System: a Density Functional Theory Study.....199
Journal of Japan Institute of Copper, 58[1] (2019) pp.23-27
E.-A. Choi, S. Z. Han, J. H. Ahn, S. Semboshi, Y. Kadoi, K. Kim and J. Lee
9. Multipole expansion for magnetic structures: A generation scheme for a symmetry-adapted orthonormal basis set in the crystallographic point group204
Phys. Rev. B, 99[17] (2019) Art.No.174407
M.-T. Suzuki, T. Nomoto, R. Arita, Y. Yanagi, S. Hayami and H. Kusunose
10. Adsorption and Diffusion of H Atoms on β -PtO₂ Surface: The Role of Nuclear Quantum Effects214
J. Phys. Chem. C, 123[22] (2019) pp.13804-13811
Yong Yang and Yoshiyuki Kawazoe
11. Understanding Hysteresis in Carbon Dioxide Sorption in Porous Metal—Organic Frameworks222
Inorg. Chem., 58[10] (2019) pp.6811-6820
Sergey A. Sapchenko, Marina O. Barsukova, Rodion V. Belosludov,
Konstantin A. Kovalenko, Denis G. Samsonenko, Artem S. Poryvaev,
Alena M. Sheveleva, Matvey V. Fedin, Artem S. Bogomyakov, Danil N. Dybtsev,
Martin Schröder and Vladimir P. Fedin
12. Spin-Orbit Coupling in All-Electron Mixed Basis Approach232
Ann. Phys., 531[9] (2019) Art.No.1900060
Takeru Nakashima and Kaoru Ohno
13. Nanoparticle Linker-Controlled Molecular Wire Devices Based on Double Molecular Monolayers241
small, 15[28] (2019) Art.No.1901183
Sohyeon Seo, Bui Quoc Viet, Eunhee Hwang, Yunhee Cho, Junghyun Lee,
Yoshiyuki Kawazoe and Hyoyoung Lee

14. Oriented Attachment Revisited: Does a Chemical Reaction Occur? 250
Matter, 1 (2019) pp.690-704
Yongfei Liu, Hongbo Geng, Xiaoying Qin, Yong Yang, Zhi Zeng,
Shuangming Chen, Yunxiang Lin, Hongxing Xin, Chunjun Song,
Xiaoguang Zhu, Di Li, Jian Zhang, Li Song, Zhengfei Dai and
Yoshiyuki Kawazoe
15. Crystal structure of η'' -Fe₃Al_{7+x} determined by single-crystal synchrotron X-ray diffraction combined with scanning transmission electron microscopy 265
Sci. Technol. Adv. Mater., 20[1] (2019) pp.543-556
Norihiko L. Okamoto, Masaya Higashi and Haruyuki Inui
16. Tip-Induced Control of Charge and Molecular Bonding of Oxygen Atoms on the Rutile TiO₂ (110) Surface with Atomic Force Microscopy 285
ACS Nano, 13[6] (2019) pp.6917-6924
Yuuki Adachi, Huan Fei Wen, Quanzhen Zhang, Masato Miyazaki,
Yasuhiro Sugawara, Hongqian Sang, Ján Brndiar, Lev Kantorovich, Ivan Štich and
Yan Jun Li
17. Pd-H and Ni-H phase diagrams using cluster variation method and Monte Carlo simulation 293
Philos. Mag., 99[19] (2019) pp.2376-2392
Natacha Bourgeois, Pierre Cenedese, Jean-Claude Crivello and
Jean-Marc Joubert
18. Reorientational motion and Li⁺-ion transport in Li₂B₁₂H₁₂ system: Molecular dynamics study 310
Phys. Rev. Mater., 3[7] (2019) Art.No.075402
Kartik Sau, Tamio Ikeshoji, Sangryun Kim, Shigeyuki Takagi, Kazuto Akagi and
Shin-ichi Orimo
19. Dehydrogenation of Methane by Partially Oxidized Tungsten Cluster Cations: High Reactivity Comparable to That of Platinum Cluster Cations 320
J. Phys. Chem. A, 123[32] (2019) pp.6840-6847
Shinichi Hirabayashi and Masahiko Ichihashi

20. Implementation of hyperfine coupling in all-electron mixed basis approach 328
J. Phys. B: At. Mol. Opt. Phys., 52[16] (2019) Art.No.165001
Hiroyuki Terada, Shota Kanno and Kaoru Ohno
21. Proposal of a new formation mechanism for hydrogenated diamond-like carbon transfer films: Hydrocarbon-emission-induced transfer 337
Carbon, 154 (2019) pp.7-12
Yang Wang, Jingxiang Xu, Yusuke Ootani, Nobuki Ozawa, Koshi Adachi and
Momoji Kubo
22. TiVZrNb Multi-Principal-Element Alloy: Synthesis Optimization, Structural, and Hydrogen Sorption Properties 343
Molecules, 24[15] (2019) Art.No.2799
Jorge Montero, Claudia Zlotea, Gustav Ek, Jean-Claude Crivello,
Lætitia Laversenne and Martin Sahlberg
23. A first-principles phase field method for quantitatively predicting multi-composition phase separation without thermodynamic empirical parameter 357
Nat. Commun., 10 (2019) Art.No.3451
Swastibrata Bhattacharyya, Ryoji Sahara and Kaoru Ohno
24. A proton transfer mechanism along the PO₄ anion chain in the [Zn(HPO₄)(H₂PO₄)]²⁻ coordination polymer 367
Phys. Chem. Chem. Phys., 21[34] (2019) pp.18605-18611
Hieu C. Dong, Hieu T. Hoang, Dinh Manh Tran, Thang B. Phan,
Sareeya Bureekaew, Yoshiyuki Kawazoe and Hung M. Le
25. Proton Conduction Inhibited by Xe Hydrates in the Water Nanotube of the Molecular Porous Crystal {[Ru^{III}(H₂bim)₃](TMA)}₂·mH₂O 374
J. Phys. Chem. C, 123[33] (2019) pp.20413-20419
Hiroshi Matsui, Tomotaka Sasaki and Makoto Tadokoro
26. Transformation of hydrogen bond network during CO₂ clathrate hydrate dissociation 381
Appl. Surf. Sci., 499 (2019) Art.No.143644
Kirill Gets, Vladimir Belosludov, Ravil Zhdanov, Yulia Bozhko,
Rodion Belosludov, Oleg Subbotin, Nikita Marasanov and Yoshiyuki Kawazoe

27. Realization of Spin-dependent Functionality by Covering a Metal Surface with a Single Layer of Molecules	388
Nano Lett., 19[10] (2019) pp.7119-7123	
H. Isshiki, K. Kondou, S. Takizawa, K. Shimose, T. Kawabe, E. Minamitani, N. Yamaguchi, F. Ishii, A. Shiotari, Y. Sugimoto, S. Miwa and Y. Otani	
28. Black phosphorene exhibiting negative thermal expansion and negative linear compressibility	393
J. Phys.: Condens. Matter, 31[46] (2019) Art.No.465003	
Lei Wang, Cong Wang and Ying Chen	
29. <i>Ab initio</i> simulations of x-ray emission spectroscopy with the <i>GW</i> +Bethe-Salpeter equation method.....	402
Phys. Rev. B, 100[7] (2019) Art.No.075149	
Tsubasa Aoki and Kaoru Ohno	
30. Atomic and Effective Pair Interactions in FeC Alloy with Point Defects: A Cluster Expansion Study	411
ISIJ Int., 59[12] (2019) pp.2343-2351	
T. Q. Nguyen, M. C. S. Escano, K. Sato, Y. Shibutani, T. Oguchi and T. Mohri	
31. Assessment of the VDW interaction converting DMAPS from the thermal-motion form to the hydrogen-bonded form.....	420
Sci. Rep., 9 (2019) Art.No.13104	
Masae Takahashi, Hiroshi Matsui, Yuka Ikemoto, Makoto Suzuki and Nobuyuki Morimoto	
32. Topology analysis for anomalous Hall effect in the noncollinear antiferromagnetic states of Mn ₃ <i>A</i> N (<i>A</i> = Ni, Cu, Zn, Ga, Ge, Pd, In, Sn, Ir, Pt)	429
Phys. Rev. B, 100[9] (2019) Art.No.094426	
Vu Thi Ngoc Huyen, Michi-To Suzuki, Kunihiko Yamauchi and Tamio Oguchi	
33. Coupling finite element method with large scale atomic/molecular massively parallel simulator (LAMMPS) for hierarchical multiscale simulations	438
Eur. Phys. J. B, 92[9] (2019) Art.No.211	
Takahiro Murashima, Shingo Urata and Shaofan Li	

34. Electron delocalization in single-layer phthalocyanine-based covalent organic frameworks: a first principle study 446
RSC Adv., 9[50] (2019) pp.29440-29447
Hung Q. Pham, Dong Q. Le, Nguyen-Nguyen Pham-Tran, Yoshiyuki Kawazoe and Duc Nguyen-Manh
35. Synergistic Effects of Nitrogen Doping on MXene for Enhancement of Hydrogen Evolution Reaction 454
ACS Sustainable Chem. Eng., 7[19] (2019) pp.16879-16888
Thi Anh Le, Quoc Viet Bui, Ngoc Quang Tran, Yunhee Cho, Yeseul Hong, Yoshiyuki Kawazoe and Hyoyoung Lee
36. Influence of the segregation of 3d transition metal solutes on the elastic modulus of a tilt grain boundary in bcc Fe: ab initio local analysis 464
J. Mater. Sci., 55[7] (2020) pp.3056-3063
Zhuo Xu, Shingo Tanaka and Masanori Kohyama
37. Phase transformation assisted twinning in a face-centered-cubic FeCrNiCoAl_{0.36} high entropy alloy 472
Acta Mater., 181 (2019) pp.491-500
Peijun Yu, Rui Feng, Junping Du, Shuhei Shinzato, Jyh-Pin Chou, Bilin Chen, Yu-Chieh Lo, Peter K. Liaw, Shigenobu Ogata and Alice Hu
38. Theoretical study of the Fe(btr)₂(NCS)₂ spin-crossover complex with reparameterized density functionals 482
Chem. Phys. Lett., 738 (2019) Art.No.136867
Saho Kajikawa and Azusa Muraoka
39. Thermodynamic anomalies and three distinct liquid-liquid transitions in warm dense liquid hydrogen 487
Phys. Rev. B, 100[13] (2019) Art.No.134109
Hua Y. Geng, Q. Wu, Miriam Marqués and Graeme J. Ackland

40. Tuning the Properties of Tetracene-Based Nanoribbons by Fluorination and N-Doping ··· 498
ChemPhysChem, 20[21] (2019) pp.2799-2805
Umer Younis, Imran Muhammad, Yoshiyuki Kawazoe and Qiang Sun
41. Triboemission of hydrocarbon molecules from diamond-like carbon friction interface induces atomic-scale wear 505
Sci. Adv., 5[11] (2019) Art.No.eaax9301
Yang Wang, Naohiro Yamada, Jingxiang Xu, Jing Zhang, Qian Chen,
Yusuke Ootani, Yuji Higuchi, Nobuki Ozawa, Maria-Isabel De Barros Bouchet,
Jean Michel Martin, Shigeyuki Mori, Koshi Adachi and Momoji Kubo
42. Synthesis of Soluble Dinaphtho[2,3-*b*:2',3'-*f*]thieno[3,2-*b*]thiophene (DNTT) Derivatives: One-Step Functionalization of 2-Bromo-DNTT 514
J. Org. Chem., 85[1] (2020) pp.195-206
Kohsuke Kawabata, Sayaka Usui and Kazuo Takimiya
43. “Disrupt and induce” intermolecular interactions to rationally design organic semiconductor crystals: from herringbone to rubrene-like pitched π -stacking 526
Chem. Sci., 11 (2020) pp.1573-1580
Chengyuan Wang, Daisuke Hashizume, Masahiro Nakano, Takuya Ogaki,
Hiroyuki Takenaka, Kohsuke Kawabata and Kazuo Takimiya
44. The role of lattice vibration in the terahertz region for proton conduction in 2D metal-organic frameworks 534
Chem. Sci., 11 (2020) pp.1538-1541
Tomoya Itakura, Hiroshi Matsui, Tomofumi Tada, Susumu Kitagawa,
Aude Demessence and Satoshi Horike
45. Raman Activity of Multilayer Phosphorene under Strain 538
ACS Omega, 4[27] (2019) pp.22418-22425
Kamil Tokár, Ján Brndiar and Ivan Štich

46. Local Density Fluctuation Governs the Divergence of Viscosity Underlying Elastic and Hydrodynamic Anomalies in a 2D Glass-Forming Liquid 546
Phys. Rev. Lett., 123[26] (2019) Art.No.265501
Hayato Shiba, Takeshi Kawasaki and Kang Kim
47. Low thermal conductivity of peanut-shaped carbon nanotube and its insensitive response to uniaxial strain 552
Nanotechnology, 31[10] (2019) Art.No.115701
Jie Sun, Kunpeng Yuan, Wenyang Zhou, Xiaoliang Zhang, Jun Onoe, Y. Kawazoe and Qian Wang
48. ミクロスケールとマクロスケールのシミュレーション連成による高分子材料系のマルチスケールシミュレーション 562
日本化学会情報化学部会誌, 37[4] (2019) pp.87-93
村島隆浩

<2020年>

1. Triphenylene and tetracene based porous sheet: Stability and electronic properties 569
Comput. Mater. Sci., 176 (2020) Art.No.109529
Imran Muhammad, Umer Younis, Huanhuan Xie, S. Ahmed, Y. Kawazoe and
Qiang Sun
2. First-principles study of Li-ion distribution at γ -Li₃PO₄/metal interfaces 576
Phys. Rev. Mater., 4 (2020) Art.No.015402
Koji Shimizu, Wei Liu, Wenwen Li, Shusuke Kasamatsu, Yasunobu Ando,
Emi Minamitani and Satoshi Watanabe
3. Graphdiyne-Based Monolayers as Promising Anchoring Materials for Lithium–Sulfur
Batteries: A Theoretical Study 586
Adv. Theory Simul., 3[3] (2020) Art.No.1900236
Imran Muhammad, Umer Younis, Huanhuan Xie, Yoshiyuki Kawazoe and
Qiang Sun
4. Multiscale Modeling of Plasticity in Amorphous & Polymeric Materials 593
IACM Expressions, 46[20] (2020) pp.10-13
S. Li, S. Urata and T. Murashima
5. True bulk As-antisite defect in GaAs(1 1 0) identified by DFT calculations and probed by
STM/STS measurements 597
Appl. Surf. Sci., 511[1] (2020) Art.No.145590
M. C. S. Escano, M. H. Balgos, T. Q. Nguyen, E. A. Prieto, E. Estacio,
A. Salvador, A. Somintac, R. Jaculbia, N. Hayazawa, Y. Kim and M. Tani
6. Crystal Structures of Dimethoxyanthracens: A Clue to a Rational Design of Packing
Structures of π -Conjugated Molecules 604
Chem. Asian. J., 15[6] (2020) pp.915-919
Kazuo Takimiya, Takuya Ogaki, Chengyuan Wang and Kohsuke Kawabata

7. Phase diagram of BaI₂-LuI₃ system and growth of BaI₂/LuI₃ eutectic scintillator 609
J. Cryst. Growth, 536 (2020) Art.No.125573
Kazuya Origuchi, Yuui Yokota, Robert Kral, Masao Yoshino, Akihiro Yamaji,
Satoshi Toyoda, Hiroki Sato, Yuji Ohashi, Shunsuke Kurosawa, Kei Kamada
and Akira Yoshikawa
8. First-Principles Study and Orbital-Fluctuation Effect on the Superconductivity in
Tungsten Bronze A_xWO₃ 614
JPS Conf. Proc., 30 (2020) Art.No.011043
Takuya Sekikawa, Rai Watabe, Jun Ishizuka, Yoshihiro Nitta, Kazuhiro Sano
and Yoshiaki Ono
9. Electronic structure of sumanene-type Buckycatcher by DFT calculations 619
Chem. Phys. Lett., 748 (2020) Art.No.137393
Azusa Muraoka and Miharu Hayashi
10. Phonon-assisted proton tunneling in the hydrogen-bonded dimeric selenates of
Cs₃H(SeO₄)₂ 624
J. Chem. Phys., 152[15] (2020) Art.No.154502
Hiroshi Matsui, Kazuki Shimatani, Yuka Ikemoto, Takahiko Sasaki and
Yasumitsu Matsuo
11. New Functionalities of Hydride Complexes with High Hydrogen Coordination 634
J. Phys. Soc. Jpn., 89[8] (2020) Art.No.051010
Shigeyuki Takagi and Shin-ichi Orimo
12. Clear evidence for element partitioning effects in a Ti-6Al-4V alloy by the first-principles
phase field method 642
J. Phys.: Condens. Matter, 32[26] (2020) Art.No.264001
Thi Nu Pham, Kaoru Ohno, Riichi Kuwahara and Swastibrata Bhattacharyya

13. First-principles analysis of the inhibitive effect of interstitial carbon on an active dissolution of martensitic steel	651
Corros. Sci., 163 (2020) Art.No.108251	
Mariko Kadowaki, Arkapol Saengdeejing, Izumi Muto, Ying Chen, Hiroyuki Masuda, Hideki Katayama, Takashi Doi, Kaori Kawano, Hideo Miura, Yu Sugawara and Nobuyoshi Hara	
14. The atomic structure of a bulk metallic glass resolved by scanning tunneling microscopy and ab-initio molecular dynamics simulation	662
J. Alloys Compd., 816 (2020) Art.No.152680	
R. V. Belosludov, A. I. Oreshkin, S. I. Oreshkin, D. A. Muzychenko, H. Kato and D. V. Louzguine-Luzgin	
15. Atomic structures and scanning tunnelling microscopy of nitrogen-doped carbon nanotubes.....	667
IOP Conf. Ser.: Mater. Sci. Eng., 744[1] (2020) Art.No.012032	
Yoshitaka Fujimoto and Susumu Saito	
16. First-Principles Approach to Water Adsorption Properties of Belite with Dopants	672
ACI Mater. J., 117[2] (2020) pp.25-32	
R. Sakurada, Y. Hosokawa, Y. Kawazoe, R. Juneja and A. K. Singh	

III. 国際会議発表論文

<Proceeding>

1. First Principle Analysis of the Effect of Strain on Electronic Transport Properties of Dumbbell-Shape Graphene Nanoribbons 681
Proc. ASME. IMECE2019, IMECE2019-11107 (2019) Art.No.V010T12A010
Takuya Kudo, Qinqiang Zhang, Ken Suzuki and Hideo Miura

2. Theoretical Study of the Edge Effect of Dumbbellshape Graphene Nanoribbon with a Dual Electronic Properties by First-principle Calculations 688
Proc. of SISPAD (2019) pp.141-144
Qinqiang Zhang, Takuya Kudo, Jowesh Gounder, Ying Chen, Ken Suzuki and Hideo Miura

<2019年>

1. Construction of Neural Network Potential to Investigate Interface Structures, Ion Migration under Electric Fields, and Phonon Properties 692
2019 Materials Research Society Spring Meeting & Exhibit
Phoenix, Arizona, USA (2019.4.22-26) No.GI01.04.09 (Poster)
Koji Shimizu, Takanori Moriya, Masayoshi Ogura, Wei Liu, Wenwen Li,
Yasunobu Ando, Emi Minamitani and Satoshi Watanabe
2. Detection of Low-lying Electronic States of Co_m^+ in He Clusters 693
International Conference on Quantum Fluid Clusters – QFC 2019
Physikzentrum Bad Honnef, Germany (2019.5.19-22) No.P18 (Poster)
M. Ichihashi and H. Odaka
3. Thermodynamic description of storage ability of nanoporous materials: Lattice dynamics and first-principles methods 694
European Materials Research Society (E-MRS) Spring Meeting
Nice, France (2019.5.27-31)
R. V. Belosludov, O. S. Subbotin, R. K. Zhdanov, Yu. Yu. Bozhko, K. V. Gets,
Y. Kawazoe and V. R. Belosludov
4. First-principles Study of Oxygen Self-diffusion and Thermal Expansion in Zirconia 695
CALPHAD XLVIII
Singapore (2019.6.2-7) No.O25
Ying Chen, Hubin Luo, Lei Wang and Tetsuo Mohri
5. Thermodynamic Stability of Substitutional Elements in Potential New Permanent Magnet Compounds $\text{R}(\text{Fe},\text{X})_{12}$ using Special Quasirandom Structures 696
CALPHAD XLVIII
Singapore (2019.6.2-7) No.O26
Arkapol Saengdeejing and Ying Chen
6. First-principles-only Phase Diagram for the Al-Ni System 697
CALPHAD XLVIII
Singapore (2019.6.2-7) No.O30
Theresa Davey, Nguyen-Dung Tran, Arkapol Saengdeejing and Ying Chen

7.	Modeling of Os-Pt System under High Hydrostatic Pressure	698
	CALPHAD XLVIII	
	Singapore (2019.6.2-7) No.O50	
	J.-M. Joubert, J.-C. Crivello and K.V. Yusenko	
8.	Identifying relaxation processes in glass-forming liquids in two dimensions	699
	25th International Congress on Glass (ICG 2019)	
	Boston, Massachusetts, USA (2019.6.9-14) No.ICG-SII-020-2019	
	Hayato Shiba, Takeshi Kawasaki and Kang Kim	
9.	Mechanisms of oxidation of pure and Si-segregated α -Ti surfaces	700
	The 14th World Conference on Titanium	
	Nantes, France (2019.6.10-14) No.T2-S7-3	
	Somesh K. Bhattacharya, Ryoji Sahara, Kyosuke Ueda and	
	Takayuki Narushima	
10.	Theoretical investigation of the phase stability and elastic properties of Ti-X alloys	701
	The 14th World Conference on Titanium	
	Nantes, France (2019.6.10-14) No.T9-S21-2	
	Ryoji Sahara, Wenchong Zhou and Koichi Tsuchiya	
11.	Construction of Neural Network Potential to Investigate Interface Structures of Au(111)/Li ₃ PO ₄	702
	The 22nd International Conference on Solid State Ionics (SSI-22)	
	PyeongChang, Korea (2019.6.16-21) No.FM-050 (Oral)	
	Koji Shimizu, Wei Liu, Wenwen Li, Yasunobu Ando, Emi Minamitani and	
	Satoshi Watanabe	
12.	Materials Informatics Based On Reliable Materials Database	703
	10th International Conference on Materials for Advanced Technologies (ICMAT 2019)	
	Marina Bay Sands, Singapore (2019.6.23-28) No.EE2-11 (Invited)	
	Yoshiyuki Kawazoe	

13. Control of Packing Structure of Thienoacene-Based Organic Semiconductors: toward “Artificial Rubrene” 704
10th International Conference on Materials for Advanced Technologies (ICMAT 2019)
Marina Bay Sands, Singapore (2019.6.23-28) (Invited)
Kazuo Takimiya
14. A Modified-CALPHAD Approach for Phase Diagrams without Experimental Data ··· 705
10th International Conference on Materials for Advanced Technologies (ICMAT 2019)
Marina Bay Sands, Singapore (2019.6.23-28) (Oral)
Theresa Davey, Nguyen-Dung Tran and Ying Chen
15. New Structure Prediction Method for Carbon Allotropes 706
10th International Conference on Materials for Advanced Technologies (ICMAT 2019)
Marina Bay Sands, Singapore (2019.6.23-28) (Oral)
Hiroshi Mizuseki and Babu Ram
16. Flat building blocks for flat silicene and the extension to 2D sheet 707
10th International Conference on Materials for Advanced Technologies (ICMAT 2019)
Marina Bay Sands, Singapore (2019.6.23-28)
Masae Takahashi
17. First-principles analysis of structure and stability in RFe₁₂-based Compounds 708
Materials Structure&Micromechanics of Fracture (MSMF9)
Brono, Czech Republic (2019.6.26-28) (Invited)
Ying Chen and Arkapol Saengdeejing
18. Ab-initio study of alloying effect of titanium and carbon on Young’s modulus of Mo₅SiB₂ (T₂) phase 709
Materials Structure&Micromechanics of Fracture (MSMF9)
Brono, Czech Republic (2019.6.26-28) (Oral)
Sojiro Uemura, Takuya Yoshida, Monika Všianská, Martin Friák, Mojmír Šob, Kyosuke Yoshimi and Sadahiro Tsurekawa

19. A new strategy for reaction path concept and dynamics effects 710
The 23rd International Annual Symposium on Computational Science and
Engineering (ANSCSE23)
Chiang Mai, Thailand (2019.6.27-29) No.CHE-I-10 (Invited)
Tetsuya Taketsugu, Takuro Tsutsumi and Yuriko Ono
20. Reaction Mechanism of the Direct Synthesis of Dimethyl Carbonate from CO₂ and
Methanol over Metal-Oxide Catalysts 711
The 23rd International Annual Symposium on Computational Science and
Engineering (ANSCSE23)
Chiang Mai, Thailand (2019.6.27-29) No.CHE-I-12 (Invited)
Akira Nakayama, Toshiyuki Sugiyama and Jun-ya Hasegawa
21. Molecular adsorption and electronic properties of doped graphene 712
The 11th International Conference on the Science and Technology for
Advanced Ceramics (STAC-11)
Tsukuba, Japan (2019.7.9-11) No.2a-405-05 (Oral)
Yoshitaka Fujimoto and Susumu Saito
22. Materials Informatics based on Reliable Materials Database 713
The 2nd Materials Research Society of Thailand International Conference
(MRS-Thailand 2019)
Pattaya, Thailand (2019.7.10-12) No.SYM11_KN01 (Keynote)
Yoshiyuki Kawazoe
23. Control of Packing Structure of Thienoacene-Based Organic Semiconductors 714
The 18th International Symposium on Novel Aromatic Compounds (ISNA-18)
Sapporo, Hokkaido, JAPAN (2019.7.21-26) No.IL-11 (Invited)
Kazuo Takimiya, Takuya Ogaki, Chengyuan Wang, Hiroyuki Takenaka and
Kohsuke Kawabata

24. Basics and Limitations in Computational Materials Design - What we should learn before starting computer simulation - 715
The 10th International Conference of the Asian Consortium on Computational Materials Science (ACCMS-10)
Hong Kong SAR (2019.7.22-26) (Invited)
Y. Kawazoe
25. Multiscale Simulation Methods in Complex Fluids 716
The 10th International Conference of the Asian Consortium on Computational Materials Science (ACCMS-10)
Hong Kong SAR (2019.7.22-26) No.WI-1-5 (Invited)
Youhei Morii and Toshihiro Kawakatsu
26. How to Realize A Reliable *Ab initio* Simulation for Materials Design Fundamentally Better than Present Day Standard 717
The 10th International Conference of the Asian Consortium on Computational Materials Science (ACCMS-10)
Hong Kong SAR (2019.7.22-26) No.WI-2-4 (Invited)
Yoshiyuki Kawazoe
27. Effects of Random Mixing and High Entropy on Stability of Promising New Permanent Magnets 718
The 10th International Conference of the Asian Consortium on Computational Materials Science (ACCMS-10)
Hong Kong SAR (2019.7.22-26) No.WI-4-6 (Invited)
Ying Chen and Arkapol Saengdeejing
28. Feasibility of the Γ point only *GW* calculation for periodic systems using TOMBO 719
The 10th International Conference of the Asian Consortium on Computational Materials Science (ACCMS-10)
Hong Kong SAR (2019.7.22-26) No.TI-1-1 (Invited)
Kaoru Ohno and Tsubasa Aoki

29. Structure-property relationship of nanoporous materials based on guest-host interaction ……720
 The 10th International Conference of the Asian Consortium on Computational Materials Science (ACCMS-10)
 Hong Kong SAR (2019.7.22-26) No.TI-2-7 (Invited)
 R. V. Belosludov
30. Methane Activation on Tungsten Compound Clusters, W_nX_m^+ …………………721
 The 10th International Conference of the Asian Consortium on Computational Materials Science (ACCMS-10)
 Hong Kong SAR (2019.7.22-26) No.TI-3-1 (Invited)
 Masahiko Ichihashi and Shinichi Hirabayashi
31. Assessment of the VDW interaction converting DMAPS from the thermal-motion form to the hydrogen-bonded form 722
 The 10th International Conference of the Asian Consortium on Computational Materials Science (ACCMS-10)
 Hong Kong SAR (2019.7.22-26) No.TI-4-3 (Invited)
 Masae Takahashi
32. Reaction Mechanism of the Direct Synthesis of Dimethyl Carbonate from CO_2 and Methanol over Metal-Oxide Catalyst: A First-Principle Study 723
 The 10th International Conference of the Asian Consortium on Computational Materials Science (ACCMS-10)
 Hong Kong SAR (2019.7.22-26) No.TI-4-10 (Invited)
 Akira Nakayama, Toshiyuki Sugiyama and Jun-ya Hasegawa
33. Theoretical and experimental study of oxidation in pure and Si-segregated α -Ti surfaces ……724
 The 10th International Conference of the Asian Consortium on Computational Materials Science (ACCMS-10)
 Hong Kong SAR (2019.7.22-26) No.FI-2-5 (Invited)
 Ryoji Sahara, Somesh Kr. Bhattacharya, Satoshi Suzuki, Kyosuke Ueda and Takayuki Narushima

34. Neural network model for predicting material properties 725
The 10th International Conference of the Asian Consortium on Computational Materials Science (ACCMS-10)
Hong Kong SAR (2019.7.22-26) No.FI-3-5 (Invited)
Hiroshi Mizuseki, Babu Ram, Ryoji Sahara and Kenta Hongo
35. Atomistic modeling of defects and precipitates in high-strength heat resistant steels 726
The 10th International Conference of the Asian Consortium on Computational Materials Science (ACCMS-10)
Hong Kong SAR (2019.7.22-26) No.WO-3-1 (Oral)
M. Souissi, M. H. F. Sluiter, T. Matsunaga, M. Tabuchi, M. J. Mills and R. Sahara
36. Phase diagram of BaI₂-LuI₃ and growth of BaI₂/LuI₃ eutectic scintillator 727
The 19th International Conference on Crystal Growth and Epitaxy (ICCGE-19)
Keystone, Colorado, USA (2019.7.28-8.2)
Kazuya Origuchi, Yuui Yokota, Robert Kral, Masao Yoshino, Akihiro Yamaji, Hiroki Sato, Yuji Ohashi, Shunsuke Kurosawa, Kei Kamada and Akira Yoshikawa
37. Role of the Acid-Base and Redox Sites on Catalytic Reactions at the Liquid/CeO₂ Interface 729
The 17th Japan-Korea symposium on molecular science "Advances in Materials and Molecular Sciences"
Nagoya, Japan (2019.7.29-31) No.S3 (Invited)
Akira Nakayama, Toshiyuki Sugiyama, Masazumi Tamura, Ken-ichi Shimizu and Jun-ya Hasegawa
38. Fermi Surface Stability Analysis in Fe-Rich Si Alloy 730
The 10th Pacific Rim International Conference on Advance Materials and Processing (PRICM-10)
Xi'an, China (2019.8.18-22) (Invited)
Ying Chen, Arkapol Saengdeejing and Tetsuo Mohri

39. Atomistic-level description of stability and composition of multicomponent clathrate hydrates 731
258th ACS National Meeting
San Diego, California, USA (2019.8.25-29)
R. V. Belosludov, Oleg S. Subbotin, Ravil K. Zhdanov, Yulia Y. Bozhko,
Kirill V. Gets, Yoshiyuki Kawazoe and Vladimir R. Belosludov
40. Theoretical study of porphyrin-based MOF structure for storage, separation and drug delivery applications 732
258th ACS National Meeting
San Diego, California, USA (2019.8.25-29)
R. V. Belosludov
41. Extended Quasiparticle Theory and Its Applications 733
Workshop on Density Functionals for Many-Particle Systems: Mathematical Theory and Physical Applications of Effective Equations
National University of Singapore (2019.9.2-6) (Invited)
Kaoru Ohno
42. Molecular Dynamics Study of Fast Li⁺ Ion Transport in Metal Borohydrides. 734
20th International Union of Materials Research Societies International Conference in Asia (IUMRS-ICA)
Perth, Australia (2019.9.22-26)
Kartik Sau, Tamio Ikeshoji, Sangryun Kim, Shigeyuki Takagi, Kazuto Akagi and Shin-ichi Orimo
43. Solvent effects of supercritical water on hydrothermal reaction: Kinetics of nickel oxide formation as a model 735
18th Asian Pacific Confederation of Chemical Engineering Congress (APCChE2019)
Sapporo, Japan (2019.9.23-27) No.F424
Akira Yoko, Yutaro Tanaka, Gimyeong Seong, Takaaki Tomai and Tadafumi Adschiri

44. Multipole expansion for magnetic structures and its application to the study of anomalous Hall effect in antiferromagnets 736
International Conference on Strongly Correlated Electron Systems 2019 (SCES2019)
Okayama Convention Center, Okayama, Japan (2019.9.23-28) (Oral)
Michi-To Suzuki, Takuya Nomoto, Ryotaro Arita, Yuki Yanagi, Satoru Hayami,
Hiroaki Kusunose, Vu Thi Ngoc Huyen, Kunihiko Yamauchi and
Tamio Oguchi
45. Rational Design of Organic Semiconductor Solid: Packing-Structure Control via Molecular Modification 737
The 14th International Conference on Cutting-Edge Organic Chemistry in Asia (ICCEOCA)
Niseko, Hokkaido, JAPAN (2019.9.26-29) No.IL-5 (Invited)
Kazuo Takimiya, Takuya Ogaki, Chengyuan Wang, Hiroyuki Takenaka and
Kohsuke Kawabata
46. Mixing and kinetics study of supercritical hydrothermal synthesis 738
The 11th International Conference on Supercritical Fluids-Supergreen 2019 (ICSF-Supergreen 2019)
Xi'an, China (2019.9.27-28) No.IL-B-07 (Invited)
Akira Yoko, Yutaro Tanaka, Gimyeong Seong, Takaaki Tomai and
Tadafumi Adschiri
47. Theoretical design of nanocatalysts for oxygen reduction and hydrogen evolution reactions 739
The 705th WE Heraeus-Seminar "Frontiers in Size-Selected Cluster Research:
Bridging the Gap"
Bad Honnef, Germany (2019.9.29-10.4)
A. Lyalin and T. Taketsugu

48. Reaction Path Concept: Intrinsic Reaction Coordinate, Anharmonic Downward Distortion Following, and Ab Initio MD 740
The ninth conference of the Asia-Pacific Association of Theoretical and Computational Chemists (APATCC2019)
Sydney, Australia (2019.9.30-10.3) No.IL019 (Invited)
Tetsuya Taketsugu, Takuro Tsutsumi, Shuichi Ebisawa and Yuriko Ono
49. ATOMISTIC LEVEL DESCRIPTION OF FUNCTIONAL MATERIALS 741
Hot Topics in Solid State Chemistry: From New Ideas to New Material (HTSSC 2019)
Novosibirsk, Russia (2019.10.1-5)
R. V. Belosludov
50. An abnormal increase in mechanical strengths at 45 and 55 mass% Ni of multicomponent Co-Ni-Cr-Mo alloys 742
The 4th International Symposium on Creation of Life Innovation Materials for Interdisciplinary and International Researcher Development (iLIM-4)
Sendai, Japan (2019.10.3-4) No.2P-18
J. Li, K. Yamanaka and A. Chiba
51. Theoretical approaches in nanocatalysis and materials design 743
Wilhelm-Ostwald-Institute for Physical and Theoretical Chemistry
Leipzig University, Leipzig, Germany (2019.10.7)
Andrey Lyalin
52. Heteroanionic surface as a new strategic approach for mitigating the side-reactions at electrolyte interface in lithium ion batteries 744
JISSE-16 Satellite Meeting
Morito Memorial Hall, Tokyo University of Science, Japan (2019.10.10-11) (Invited)
Nobuyuki Zettsu and Katsuya Teshima

53. First-Principles Investigation of the Effect of Interstitial Carbon on Corrosion Resistance of Martensitic Medium-Carbon Steel 746
236th ECS Meeting
Atlanta, GA, USA (2019.10.13-17) No.C04-0866
Mariko Kadowaki, Arkapol Saengdeejing, Izumi Muto, Ying Chen,
Hiroyuki Masuda, Hideki Katayama, Takashi Doi, Kaori Kawano,
Hideo Miura, Yu Sugawara and Nobuyoshi Hara
54. Toward “Designed Organic Semiconductors”: Manipulation of Packing Structures by Molecular Design 747
13rd Japan-China Joint Symposium on Conduction and Photoconduction in Organic Solids and Related Phenomena (13JS)
Shanghai, China (2019.10.20-23) No.IL-76 (invited)
Kazuo Takimiya, Chengyuan Wnag, Hiroyuki Takenaka, Takuya Ogaki and Kohsuke Kawabata
55. Effect of Surface Oxysulfidation on LiNi_{0.5}Mn_{1.5}O₄ Single Crystals Shapesand Their Electrochemical Characterization 748
The 13th Pacific Rim Conference of Ceramic Societies (PACRIM13)
Okinawa Convention Center, Japan (2019.10.27-11.1) No.31-A2-S20-35 (Oral)
Nobuyuki Zettsu, Dae-wook Kim, Hiromasa Shiiba and Katsuya Teshima
56. Theory of single spin spectroscopy at surfaces: from Kondo singlet to spin-orbit interaction 749
Exploring the Limits of Nanoscience with Scanning Probe Methods
Physikzentrum Bad Honnef, Germany (2019.10.27-31)
Emi Minamitani
57. Investigation of Interface Structures of Au(111)/Li₃PO₄ using High-Dimensional Neural Network Potential 750
The 22nd Asian Workshop on First-Principles Electronic Structure Calculations (ASIAN-22)
Koji Shimizu, Wei Liu, Wenwen Li, Yasunobu Ando, Emi Minamitani and Satoshi Watanabe

58. Diffusion of Carbon in α -Fe in the Presence of Vacancy 751
The 22nd Asian Workshop on First-Principles Electronic Structure Calculations
(ASIAN-22)
Osaka University Hall, Osaka, Japan (2019.10.28-30)
Tien Quang Nguyen, Ngoc Nam Ho, Kazunori Sato and Yoji Shibutani
59. Excited-state branching reaction of stilbene derivatives 752
2019 International Conference on Theoretical and High Performance Computational
Chemistry (ICT-HPCC19)
Guiyang, China (2019.11.2-5)
Tetsuya Taketsugu, Yu Harabuchi, Takuro Tsutsumi, Rina Yamamoto and
Satoshi Maeda
60. Electronic states of Al-Mg-Zn quasicrystal and its approximant based on the
first-principles calculations 753
14th International Conference on the Structure of Non-Crystalline Materials
Kobe, Japan (2019.11.3-8) No.P48
Masaki Saito, Takuya Sekikawa and Yoshiaki Ōno
61. Determination of the Localized-to-extended-state Transition Point of the Metal-insulator
Transition of Fluid Mercury using Multifractal Analysis 754
14th International Conference on the Structure of Non-Crystalline Materials
Kobe, Japan (2019.11.3-8) No.P50
K. Kobayashi, T. Sekikawa and K. Maruyama
62. Theoretical design of flat silicene molecules towards flat 2D silicene sheets 755
The 5th International Conference on Molecular Simulation (ICMS 2019)
Lotte Hotel Jeju, Korea (2019.11.3-6) (Invited)
Masae Takahashi
63. Neural Network Prediction on High-entropy Alloys 756
The 5th International Conference on Molecular Simulation (ICMS 2019)
Lotte Hotel Jeju, Korea (2019.11.3-6) No.Or-T02-131 (Oral)
Hiroshi Mizuseki, Babu Ram, Ryoji Sahara and Kenta Hongo

64. First-principles investigation to improve the stability of β - and β' -Cu₄Ti precipitates in Cu-Ti alloy 757
The 5th International Conference on Molecular Simulation (ICMS 2019)
Lotte Hotel Jeju, Korea (2019.11.3-6) No.Or-T04-315 (Oral)
E.-A. Choi, S. Z. Han, J. Ahn, S. H. Lim and S. Semboshi
65. Implementation of high-performance effective-field-calculation algorithm for ultra-large-scale micromagnetic simulation on multi-GPUs 758
The 64th Annual Conference on Magnetism and Magnetic Materials (2019MMM)
Las Vegas, NV, USA (2019.11.4-8) No.FI-09
H. Tsukahara and K. Ono
66. Theoretical design of novel catalytic materials using SIESTA 759
Japan Association for Chemical Innovation (JACI)
Tokyo, Japan (2019.11.8)
Andrey Lyalin
67. Conceptual design of multi-functional nanomaterials based on porphyrin subunits 760
ACS Publications Symposium: Innovation in Materials Science and Technology
Singapore (2019.11.17-19)
R. V. Belosludov
68. Theoretical elucidation of photo-reaction mechanism: applications to stilbene derivatives 761
The 15th Nanjing University-Hokkaido University-NIMS Joint Symposium
Nanjing, China (2019.11.24-26) No.O-06
Tetsuya Taketsugu
69. Synthetic method for 6,13-dihydoroxyquinacridone via difluoroboron chelation to quinacridonequinone 763
The 3rd FRIMS International Symposium on Frontier Materials
Nagoya, Japan (2019.11.25-26) No.P34
Masayuki Takeda, Koichiro Moriya and Katsuhiko Ono

70. Trend of Human Resource Development in Doctorate Holders in Computational Materials Science in Japan 764
SMS2019 & GIMRT User Meeting 2019
Sendai, Japan (2019.11.27-29)
Yayoi Terada and Tetsuo Mohri
71. Supercomputer Simulation of Atomic Scale Friction for Design of Sliding Materials 765
GIMRT X ISS-"Kibo" Users' Network X AIRC ~International Collaborative Research Platform on Ground and in Orbit~
Sendai, Japan (2019.11.29) (Invited)
Y. Ootani, Y. Wang and M. Kubo
72. Theoretical study on Tandem Solar Cell Configuration based on different Si allotropes 766
MRS Fall Meeting
Boston, Massachusetts, USA (2019.12.1-6)
R. V. Belosludov and H. Morito
73. Changes in the number of doctoral degree holders in computational materials science in Japan during the last 50 years -Text data mining analysis on the difference between research universities and education-oriented universities- 767
MRS Fall Meeting
Boston, Massachusetts, USA (2019.12.1-6)
Yayoi Terada and Tetsuo Mohri
74. Order parameter and Topological features for Large Anomalous Hall Effect 768
International Conference on Topological Materials Science 2019 (Topomat2019)
Kyoto University, Kyoto, Japan (2019.12.3-7) (Oral)
M.-T. Suzuki, V. T. N. Huyen, K. Yamauchi, T. Oguchi, T. Nomoto, R. Arita,
Y. Yanagi, S. Hayami and H. Kusunose

75.	Construction of Neural Network Potential to Investigate Interface Structures of Au(111)/Li ₃ PO ₄	769
	Materials Research Meeting 2019	
	Yokohama, Japan (2019.12.10-14) (Oral)	
	Koji Shimizu, Wei Liu, Wenwen Li, Yasunobu Ando, Emi Minamitani and Satoshi Watanabe	
76.	A prototype first-principles only phase diagram: Al-Ni	770
	Materials Research Meeting 2019	
	Yokohama, Japan (2019.12.10-14) No.A3-11-O02 (Oral)	
	Theresa Davey, Nguyen-Dung Tran, Arkapol Saengdeejing and Ying Chen	
77.	Thermodynamic Stability Study of Substitutional Elements in (R,M)(Fe,X) ₁₂ Structure using Special Quasirandom Structures	771
	Materials Research Meeting 2019	
	Yokohama, Japan (2019.12.10-14) No.E1-13-O03 (Oral)	
	Arkapol Saengdeejing and Ying Chen	
78.	Micromagnetic simulation of magnetization reversals and domain wall motions inside permanent magnet	772
	Materials Research Meeting 2019	
	Yokohama, Japan (2019.12.10-14) No.E1-13-O10 (Oral)	
	Hiroshi Tsukahara, Kaoru Iwano, Tadashi Ishikawa, Chiharu Mitsumata and Kanta Ono	
79.	Molecular Dynamics Study of Fast Li ⁺ Ion Transport in <i>clos</i> -Boranes.	773
	Materials Research Meeting 2019	
	Yokohama, Japan (2019.12.10-14) No.A2-12-O03 (Oral)	
	Kartik Sau, Tamio Ikeshoji, Sangryun Kim, Shigeyuki Takagi, Kazuto Akagi and Shin-ichi Orimo	
80.	Hydride Complexes with High Hydrogen Coordination and Their Novel Functionalities	774
	Materials Research Meeting 2019	
	Yokohama, Japan (2019.12.10-14) No.A2-13-O08 (Oral)	
	S. Takagi and S. Orimo	

81. Molecular adsorption and electronic properties of doped graphene for sensing applications 775
Materials Research Meeting 2019
Yokohama, Japan (2019.12.10-14) No.D1-11-O04 (Oral)
Yoshitaka Fujimoto and Susumu Saito
82. Electronic properties of graphene/C-doped h-BN heterostructures 776
Materials Research Meeting 2019
Yokohama, Japan (2019.12.10-14) No.D1-13-O08 (Oral)
Taishi Haga, Yoshitaka Fujimoto and Susumu Saito
83. First-principles prediction of magnetic structures in crystal 777
Materials Research Meeting 2019
Yokohama, Japan (2019.12.10-14) No.B1-12-P14 (Poster)
Michi-To Suzuki and Yuki Yanagi
84. Electronic Structure of Periodically Modified Graphene 778
Materials Research Meeting 2019
Yokohama, Japan (2019.12.10-14) No.D1-11-P04 (Poster)
Tomoya Ito and Susumu Saito

<2020年>

1. Theoretical Materials Research in Past and Future 779
International Conference on Materials Genome (ACCMS-ICMG 2020)
Amaravati, INDIA (2020.2.5-7) No.IL-2 (Invited)
Y. Kawazoe
2. Machine Learning on Band Gap Prediction of III-V Compound Semiconductor 780
International Conference on Materials Genome (ACCMS-ICMG 2020)
Amaravati, INDIA (2020.2.5-7) No.IL-12: (Invited)
Hiroshi Mizuseki
3. Molecular spins at surfaces: from Kondo singlet to application for spintronics 781
The 3rd Symposium for The Core Research Clusters for Materials Science and
Spintronics
Sendai International Center, Sendai, Japan (2020.2.10-11) No.12-B
Emi Minamitani
4. Text Data Mining Analysis on Changes in the Number of Doctoral Degree Holders in
Computational Materials Science in Japan during the Last 50 Years 782
TMS 2020 Annual Meeting & Exhibition
San Diego, California, USA (2020.2.23-27) No.L-35
Yayoi Terada and Tetsuo Mohri
5. High Entropy Alloy Effect on Stability of Potential Permanent Magnets 783
TMS 2020 Annual Meeting & Exhibition
San Diego, California, USA (2020.2.23-27)
Ying Chen and Arkapol Saengdeejing
6. Reduction of Uncertainty in a First-principles-based CALPHAD-type Phase Diagram via
Sequential Learning of Phase Equilibrium Data 784
TMS 2020 Annual Meeting & Exhibition
San Diego, California, USA (2020.2.23-27)
Theresa Davey, Brandon J. Bocklund, Zi-Kui Liu and Ying Chen

7. Thermodynamic of Multicomponent Gas Hydrate Systems: Theoretical Aspects 785
Natural Gas Hydrate Systems Gordon Research Conference
Galveston, TX, USA (2020.2.23-28)
R. V. Belosludov, K. V. Gets, R. K. Zhdanov, Yu. Yu. Bozhko and
V. R. Belosludov
8. Atomistic Kinematics of Carbon Diffusion and Clustering in BCC Fe with Point
Defects 786
APS March Meeting 2020
Colorado Convention Center, Denver, Colorado, USA (2020.3.2-6)
Tien Quang Nguyen, Kazunori Sato and Yoji Shibutani

IV. 予稿集

<Proceeding>

1. Atomistically Kinetic Simulations of Carbon Diffusion in α -Fe with Point Defect 787
The Proceedings of The Computational Mechanics Conference, 32 (2019)
Art.No.250
T. Q. Nguyen, N. N. Ho, K. Sato and Y. Shibutani

<2018年>

1. 微量成分で置換したビーライトの水分子吸着エネルギー 791

平成30年度土木学会東北支部技術研究発表会

東北大学川内北キャンパス (2019.3.2) No.V-11

桜田良治、細川佳史、川添良幸、鶴澤正美、Abhishek Kumar Singh

<2019年>

1. Theoretical design of porphyrin-based nanostructures 793
ナノ学会第17回大会
かごしま県民交流センター (2019.5.9-11) No.O-11 (Oral)
Rodion V. Belosludov、川添良幸
2. ドープした炭素ナノ構造体中のポーラロン 794
ナノ学会第17回大会
かごしま県民交流センター (2019.5.9-11) No.O-15 (Oral)
川添良幸
3. クラスター複合体の赤外光解離分光 795
第21回理論化学討論会
ナノ学会第17回大会
かごしま県民交流センター (2019.5.9-11) No.O-35 (Oral)
市橋正彦、尾高英穂
4. 部分的に酸化されたタングステンクラスター正イオンによるメタンの活性化 796
ナノ学会第17回大会
かごしま県民交流センター (2019.5.9-11) No.P-46 (Poster)
平林慎一、市橋正彦
5. Application of First-Principles Potential Renormalization Theory to a Phase Transition between bcc and fcc Fe Crystals 797
ナノ学会第17回大会
かごしま県民交流センター (2019.5.9-11) No.P-49 (Poster)
Thi Nu Pham, Ryoji Sahara, Riichi Kuwahara and Kaoru Ohno
6. Cs₃H(SeO₄)₂ の異常なフォノンとプロトンの相関 798
日本固体イオニクス学会第22回超イオン導電体物性研究会
沖縄県青年会館 (2019.5.25-26)
松井広志、島谷和紀、池本夕佳、松尾康光

7. AI による未来～電子デバイス設計への適用～ 802
NEDIA Day 東北みやぎ
片平さくらホール (2019.8.1)
川添良幸
8. 混相流のマルチスケール解析に関するサブ課題 B での連携研究 803
第3回ポスト「京」萌芽的課題「基礎科学の挑戦」・「極限マテリアル」合
同公開シンポジウム
東北大学金属材料研究所 (2019.8.1)
森井洋平、村島隆浩、川勝年洋、芝隼人、寺田弥生、谷口貴志、
山本量一、國嶋雄一、松田景吾、大西領、浅野優太、渡辺宙志、
野口博司、小屋口剛博、伊藤伸泰、本田隆
9. 局所エネルギー・局所応力の第一原理計算法開発：類似手法との比較と金属粒
界への適用 804
日本物理学会 2019 年秋季大会
岐阜大学(柳戸キャンパス) (2019.9.10-13) No.12pB22-1
香山正憲、徐卓、田中真悟、椎原良典
10. Xe を内包した水ナノチューブのプロトン伝導 805
日本物理学会 2019 年秋季大会
岐阜大学(柳戸キャンパス) (2019.9.10-13) No.12pK37-8
松井広志、佐々木智崇、佐久間惇、田所誠
11. 二次元の各種ブラベー格子の周期で構造修飾されたグラフェンの電子構造 806
日本物理学会 2019 年秋季大会
岐阜大学(柳戸キャンパス) (2019.9.10-13) No.13pD15-4
伊藤智哉、斎藤晋
12. η -Fe₂Al₅相単結晶熱電特性の結晶方位依存性 807
日本金属学会 2019 年秋期(第 165 回)講演大会
岡山大学津島キャンパス (2019.9.11-13) No.32
藤原浩輔、岡本範彦、市坪哲

13. *Ab initio* local analysis on the stability of Mg symmetric tilt grain boundaries 808
日本金属学会 2019 年秋期(第 165 回)講演大会
岡山大学津島キャンパス (2019.9.11-13) No.296
Zhuo XU, Masanori KOHYAMA and Singo TANAKA
14. 第一原理計算を用いたマルテンサイト鋼の耐食性におよぼす固溶炭素の影響
解明 809
日本金属学会 2019 年秋期(第 165 回)講演大会
岡山大学津島キャンパス (2019.9.11-13) No.403
門脇万里子、Arkapol Saengdeejing、武藤泉、陳迎、升田博之、片山英樹、
土井教史、河野佳織、三浦英生、菅原優、原信義
15. 白金族金属酸化物クラスター正イオンとメタンとの反応 810
第 13 回分子科学討論会
名古屋大学東山キャンパス (2019.9.17-20) No.3B01 (Oral)
平林慎一、市橋正彦
16. タングステン酸化物クラスター上でのメタンの活性化 812
第 124 回触媒討論会
長崎大学文教キャンパス (2019.9.18-20) No.1F12 (Oral)
市橋正彦、平林慎一
17. 鉛フリー有機無機ペロブスカイトの電子状態計算 813
第 80 回応用物理学学会秋季学術講演会
北海道大学札幌キャンパス (2019.9.18-21) No.20a-PB2-12
井手敦子、山本久美子、奥村峻、飯久保智、早瀬修二
18. 有機半導体の結晶構造制御：小官能基による分子間相互作用への影響 814
2019 年度化学系学協会東北大会
山形大学小白川キャンパス (2019.9.21-22) No.21B1 (依頼講演)
瀧宮和男

19. キナクリドンキノンへのホウ素キレート化による 6,13-ジヒドロキシキナクリドンの合成 815
第 30 回基礎有機化学討論会
大阪国際交流センター (2019.9.25-27) No.1B06 (Oral)
小野克彦、森谷晃一朗、島田涼平
20. Effects of microstructure on magnetization reversal inside hot-deformed permanent magnet 816
第 43 回日本磁気学会学術講演会
京都大学吉田キャンパス (2019.9.25-27) No.25pA-2
H. Tsukahara, K. Iwano, C. Mitsumata, T. Ishikawa and K. Ono
21. Possible Design and Development of Ultra-high Strength Permanent Magnet Based on Fundamental Conceptual Change in Magnetism 817
第 43 回日本磁気学会学術講演会
京都大学吉田キャンパス (2019.9.25-27) No.26aA-2
Yoshiyuki Kawazoe
22. 高分子を含む複雑流動のマルチスケールシミュレーション 818
第 68 回高分子討論会
福井大学文京キャンパス (2019.9.25)
森井洋平、川勝年洋
23. Stability calculation of Cu₄Ti intermetallic compound with addition of 3d transition metal in Cu-Ti alloy by density functional theory 821
日本銅学会第 59 回講演大会
関西大学千里山キャンパス (2019.10.19-20)
E.-A. Choi, S. Z. Han, J. Ahn, S. Semboshi, J. Lee and S. H. Lim
24. 過去 50 年間の国内の計算物質科学分野の博士号取得者数の推移 823
PCoMS シンポジウム & 計算物質科学スーパーコンピュータ共用事業報告会 2019
東北大学片平キャンパス (2019.10.24-25)
寺田弥生、毛利哲夫

25. PCoMS 合宿セミナー実施報告 824
PCoMS シンポジウム & 計算物質科学スーパーコンピュータ共用事業報告会 2019
東北大学片平キャンパス (2019.10.24-25)
寺田弥生、川勝年洋、毛利哲夫
26. マルチスケール流動シミュレーション用プラットフォームの開発 825
PCoMS シンポジウム & 計算物質科学スーパーコンピュータ共用事業報告会 2019
東北大学片平キャンパス (2019.10.24-25)
村島隆浩、森井洋平、川勝年洋
27. Atomistic simulations of carbon behavior in BCC iron with point defects 826
PCoMS シンポジウム & 計算物質科学スーパーコンピュータ共用事業報告会 2019
東北大学片平キャンパス (2019.10.24-25)
Tien Quang NGUYEN, Kazunori SATO and Yoji SHIBUTANI
28. 複雑流動のマルチスケールシミュレーション 827
セミナーシリーズ 「スパコンプロフェッショナル No.24」
東北大学金属材料研究所 (2019/10/29)
森井洋平、川勝年洋
29. Li₄Ti₅O₁₂ 結晶の複合アニオン表面化による機能創発 828
第 60 回電池討論会
国立京都国際会館 (2019.11.13.-15) No.1B07
是津信行、キムヘミン、キムデウク、椎葉寛将、原健治朗、手嶋勝弥
30. Molecular Simulations of Ionic-Liquid-based Electrical Double Layer Capacitors 829
第 10 回イオン液体討論会
大阪府豊中市 (2019.11.21) No.1O04
Patrick Bonnau and Hayato Shiba

31. Au(111)/Li₃PO₄ の界面構造探索に向けたニューラルネットワークポテンシャルの構築 831
第45回固体イオニクス討論会
九州大学伊都キャンパス椎木講堂 (2019.11.26-28) No.1A-11 (Oral)
清水康司、Wei Liu、Wenwen Li、安藤康伸、南谷英美、渡邊聰
32. Carbon diffusion and clustering in bcc iron: A kinetic Monte Carlo study 833
Workshop on Nanotechnology-Driven Topics
Osaka University, Osaka, Japan (2019.12.10)
Tien Quang Nguyen, Kazunori Sato and Yoji Shibutani
33. 2次元ガラス形成液体の粘弾性特性と緩和過程 834
第33回分子シミュレーション討論会
名古屋市昭和区 (2019.12.11) No.303S
芝隼人、川崎猛史、金鋼
34. 錯体水素化物固体電解質の開発 835
電気化学会東北支部 第50回セミコンファレンス
山形県天童市 (2019.12.15-16)
高木成幸

<2020年>

1. 水ナノチューブにおける Xe 水和物生成とプロトン伝導の抑制効果 836
ウォーターフロンティアサイエンス&テクノロジー研究センター研究成果
報告会
東京理科大学葛飾キャンパス図書館ホール (2020.1.25)
松井広志
2. マルチスケール流動シミュレーション用プラットフォーム (MSSP) の開発、
および、複雑流動のシミュレーション 838
第9回材料系ワークショップ～「富岳」で飛躍へ！計算データの価値～
秋葉原コンベンションホール (2020.2.17) No.P35
川勝年洋
3. 近赤外光解離分光による極低温コバルトクラスターイオンの電子構造の解明 839
日本物理学会第75回年次大会
名古屋大学 (2020.3.16-19) No.19aK26-9 (現地開催中止)
尾高英穂、市橋正彦
4. SiO₂における Cristobalite 構造の安定性に関する第一原理計算 840
日本金属学会 2020年春期(第166回)講演大会
東京工業大学大岡山キャンパス (2020.3.17-19) No.143 (現地開催中止)
陳迎、Tran Nguyen-Dung、北岡諭、毛利哲雄
5. 第一原理フェーズフィールド法による合金組織の予測技術 841
日本金属学会 2020年春期(第166回)講演大会
東京工業大学大岡山キャンパス (2020.3.17-19) No.150 (現地開催中止)
大野かおる、Swastibrata Bhattacharyya、佐原亮二、Thi Nu Pham、
桑原理一
6. Study of alloying element effects on the microstructure in Ti alloys using
first-principles phase field method 842
日本金属学会 2020年春期(第166回)講演大会
東京工業大学大岡山キャンパス (2020.3.17-19) No.151 (現地開催中止)
"Thi Nu Pham, Kaoru Ohno, Riichi Kuwahara, Ryoji Sahara and
Swastibrata Bhattacharyya

7. 日本の計算物質科学とマテリアルズインフォマティクスの博士号取得者数の近年の推移に対する考察 843
　　日本金属学会 2020 年春期(第 166 回)講演大会
　　東京工業大学大岡山キャンパス (2020.3.17-19) No.360 (現地開催中止)
　　寺田弥生、毛利哲夫
8. 9 配位錯イオンを含む錯体水素化物におけるリチウムイオン輸送特性 844
　　日本金属学会 2020 年春期(第 166 回)講演大会
　　東京工業大学大岡山キャンパス (2020.3.17-19) No.412 (現地開催中止)
　　高木成幸、池庄司民夫、折茂慎一
9. Cluster Variation Calculations of Pair Probabilities in Multicomponent Alloy: Application to the FCC Cr-Fe-Mn-Ni System 845
　　日本金属学会 2020 年春期(第 166 回)講演大会
　　東京工業大学大岡山キャンパス (2019.3.20-19) No.fcc (現地開催中止)
　　Tien Quang NGUYEN, Mary Clare Sison ESCANO, Kazunori SATO,
　　Yoji SHIBUTANI, Tamio OGUCHI and Tetsuo MOHRI
10. Stability of Ternary Subsystems of FeNiCoCrMn/Pd High Entropy Alloys: A First Principles Study 846
　　日本金属学会 2020 年春期(第 166 回)講演大会
　　東京工業大学大岡山キャンパス (2020.3.17-19) No.P91 (現地開催中止)
　　Tran Nguyen- Dung and Ying Chen
11. 直線形ドナー-π-アクセプタ構造を与えるボロン β-ケトイミネート色素の合成と太陽電池特性 847
　　日本化学会第 100 春季年会 (2020)
　　東京理科大学野田キャンパス (2020.3.22-25) No.2C3-12 (Oral) (現地開催中止)
　　小野克彦、佐倉裕規、弓岡史奈

V. 新聞記事

<2019年>

1. ファンデルワールス力の発現 テラヘルツ光と放射光で測定
科学新聞 (2019.10.4) (目次のみ掲載)

VI. 学位取得

1. シアル酸水和の振動吸収スペクトルへの影響

東北大学大学院農学研究科生物産業創成科学専攻
食品機能健康科学講座テラヘルツ生物工学研究室
富春亜

2. Efeito de uma zona de exclusão ao redor dos núcleos na transformação de fase

Universidade Federal Fluminense, Núcleo de Modelamento Microestrutural,
Microstructural Modeling Group
Harison da Silva Ventura

3. Simulação computacional de transformações com nucleação e velocidade não homogêneas

Universidade Federal Fluminense, Núcleo de Modelamento Microestrutural,
Microstructural Modeling Group
Mariana Sizenando Lyrio

VII. その他

1. 本所情報関係委員会メンバー・学内情報関連委員 849
2. 東北大学金属材料研究所構内図 850
3. スーパーコンピューターシステム関連 レイアウト図 851