

## センター利用による研究成果

—平成 28 年度計算機利用結果報告書から—

### 【1002 ソフトウェア】

1. Tatsuya Abe, Tomoharu Ugawa, Toshiyuki Maeda, and Kousuke Matsumoto : Reducing State Explosion for Software Model Checking with Relaxed Memory Consistency Models : Proceedings of the 2nd International Symposium on Dependable Software Engineering: Theories, Tools and Applications, Vol.LNCS9984, pp.118-135, 2016

### 【4304 数理物理・物性基礎】

2. Yosuke Harashima, Kiyoyuki Terakura, Hiori Kino, Shoji Ishibashi and Takashi Miyake : First-principles study on stability and magnetism of NdFe<sub>11</sub>M(N) for M=Ti, V, Cr, Mn, Fe, Co, Ni, Cu, Zn : Journal of Applied Physics, Vol.120, pp.203964-1 - 203964-6, 2016
3. Yosuke Harashima, Kiyoyuki Terakura, Hiori Kino, Shoji Ishibashi, and Takashi Miyake : Nitrogen as the best interstitial dopant among X = B, C, N, O, and F for strong permanent magnet NdFe<sub>11</sub>TiX: First-principles study : Physical Review B, Vol.92, pp.184426-1 - 184426-13, 2015

### 【4306 生物物理・化学物理】

4. Shun Sakuraba, Hidetoshi Kono : Spotting the difference in molecular dynamics simulations of biomolecules : The Journal of the Chemical Physics, Vol.145, pp.074116 - , 2016
5. Hirotaka Kitoh-Nishioka, Koji Ando : FMO3-LCMO study of electron transfer coupling matrix element and pathway: Application to hole transfer between two tryptophans through cis- and trans-polyproline-linker systems : The Journal of

Chemical Physics, Vol.145, pp.114103 - , 2016

6. Hirotaka Kitoh-Nishioka, Daisuke Yokogawa, and Stephan Irle: Forster Resonance Energy Transfer between Fluorescent Proteins: Efficient Transition Charge-Based Study : The Journal of Physical Chemistry C, Vol.121, No.8, pp.4220-4238, 2017
7. Hirotaka Kitoh-Nishioka, Kai Welke, Yoshio Nishimoto, Dmitri G. Fedorov, and Stephan Irle : Multiscale Simulations on Charge Transport in Covalent Organic Frameworks Including Dynamics of Transfer Integrals from the FMO-DFTB/LCMO Approach : The Journal of Physical Chemistry C, Vol.121, No.33, pp.17712-17726, 2017

### 【4501 プラズマ科学】

8. Miyake, Y., H. Usui : Particle-in-cell modeling of spacecraft-plasma interaction effects on double-probe electric field measurements : Radio Science, Vol.51, pp.1905 - 1922, 2016

### 【4601 物理化学】

9. Yoshio Nishimoto and Dmitri G. Fedorov : Three-Body Expansion of the Fragment Molecular Orbital Method Combined with Density-Functional Tight-Binding : Journal of Computational Chemistry, Vol.38, No.7, pp.406 - 418, 2017
10. M. Hatanaka, Y. Hirai, Y. Kitagawa, T. Nakanishi, Y. Hasegawa, K. Morokuma : Organic linkers control the thermosensitivity of the emission intensities from Tb(III) and Eu(III) in a chameleon polymer : Chemical Science, Vol.8, pp.423-429, 2016
11. Yoshio Nishimoto : Analytic Hyperpolarizability and polarizability

- derivative with fractional occupation numbers for large extended systems : The Journal of Chemical Physics, Vol.146, No.8, pp.084101-, 2017
- 【4704 機能物質化学】
12. D. V. Konarev, Y. Nakano, S. S. Khasanov, A. V. Kuzmin, M. Ishikawa, A. Otsuka, H. Yamochi, G. Saito, R. N. Lyubovskaya : Magnetic and optical properties of layered (Me4P+)[M(IV)O(Pc•3-)]•- (TPC)0.5 C6H4Cl2 salts (M = Ti and V) composed of  $\pi$ -stacking dimers of titanyl and vanadyl phthalocyanine radical anions : Cryst. Growth Des., Vol.17, No.2, pp.753-762, 2016
  13. D. V. Konarev, S. I. Troyanov, A. V. Kuzmin, Y. Nakano, M. Ishikawa, M. A. Faraonov, S. S. Khasanov, A. L. Litvinov, A. Otsuka, H. Yamochi, G. Saito, R. N. Lyubovskaya : The Salts of Copper Octafluoro- and Hexadecafluorophthalocyanines Containing [CuII(F8Pc)4-]2- Dianions and [CuF16Pc]- Monoanions : Inorg. Chem., Vol.56, No.4, pp.1804-1813, 2017
  14. D. V. Konarev, S. S. Khasanov, M. Ishikawa, Y. Nakano, A. Otsuka, H. Yamochi, G. Saito, R. N. Lyubovskaya : Tetrabutylammonium salts of aluminum(III) and gallium(III) phthalocyanine radical anions bonded with fluoren-9-olato- anions and indium(III) bromide phthalocyanine radical anions : Chem. Asian J., Vol.12, 2017
  15. 中野義明, 大江佳毅, 石川学, 矢持秀起, 売市幹大 : 3回対称性ドナー分子を用いた電荷移動錯体の合成と物性評価 (ポスター発表) : 第10回分子科学討論会 2016 神戸, 2016
  16. 中野義明, 大江佳毅, 石川学, 矢持秀起, 売市幹大 : 3回対称性分子と TCNQ からなる電荷移動錯体の作製と物性評価 (ポスター発表) : 京都大学物性科学センター第15回講演会・研究交流会, 2017
  17. Y. Nakano, Y. Oe, M. Ishikawa, H. Yamochi, M. Uruichi : Development of Organic Electronics Material Based on C3-Symmetric Molecule (ポスター発表) : 12th International Conference on Nano-Molecular Electronics (ICNME2016), 2016
- 【4801 機能材料・デバイス】
18. Genta Kawaguchi, Mitsuhiko Maesato, Tokutaro Komatsu, Tatsuro Imakubo, Andhika Kiswandhi, D. Graf, Hiroshi Kitagawa : Use of Halogen Bonding in a Molecular Solid Solution to Simultaneously Control Spin and Charge : Chemistry of Materials, Vol.28, No.20, pp.7276 - 7286, 2016
  19. Mikihiro Hayashi, Kazuya Otsubo, Mitsuhiko Maesato, Tokutaro Komatsu, Kuniyoshi Sugimoto, Akihiro Fujiwara, Hiroshi Kitagawa : An Electrically Conductive Single-Component Donor-Acceptor-Donor Aggregate with Hydrogen-Bonding Lattice : Inorganic Chemistry, Vol.55, No.24, pp.13027 - 13034, 2016
  20. Tokutaro Komatsu, Hirokazu Kobayashi, Kohei Kusada, Yoshiki Kubota, Masaki Takata, Tomokazu Yamamoto, Syo Matsumura, Katsutoshi Sato, Katsutoshi Nagaoka, Hiroshi Kitagawa : First-Principles Calculation, Synthesis and Catalytic Properties of Rh-Cu Alloy Nanoparticles : Chemistry - A European Journal, Vol.23, No.1, pp.57 - 60, 2016
  21. Natalia Palina, Osami Sakata, L. S. R. Kumara, Chulho Song, Katsutoshi Sato, Katsutoshi Nagaoka, Tokutaro Komatsu, Hirokazu Kobayashi, Kohei Kusada & Hiroshi Kitagawa : Electronic Structure Evolution with Composition Alteration of RhxCuy Alloy Nanoparticles : Scientific Reports, Vol.7, pp.41264-, 2017
- 【4904 応用物理学一般】
22. Tien-Hsiu Tsai and Ikuo Kanno : A simulation study on the influence of scattered X-rays in energy-resolved computed tomography : Journal of Nuclear Science and Technology, Vol.54, No.2, pp.205-212, 2016
- 【4905 工学基礎】

23. Shugo YASUDA: Monte Carlo simulation for kinetic chemotaxis model: an application to the traveling population wave : *Journal of Computational Physics*, Vol.330, pp.1022-1042, 2016
- 【5001 機械材料・材料力学】
24. 西川雅章, 内藤悠太, 金崎真人, 北條正樹: 炭素繊維熱可塑性複合材料の加熱成形プロセスに関する熱伝導特性と粘弾性変形の連成解析 : *JCOM 若手シンポジウム 講演論文集*, 2016
25. Masaaki Nishikawa, Akira Fukuzo, Naoki Matsuda, Masaki Hojo : Load-Transfer-Based Micromechanical Simulation for Evaluating Elastic-Plastic Response of Discontinuous Carbon Fiber Reinforced Thermoplastics : *Proc. of 31st Technical Conference of American Society for Composites*, 2016
26. 古賀貢史, 新玉重貴, 西川雅章, 北條正樹, 松田直樹: ボイドを含む CFRP の層間せん断試験の樹脂の降伏を考慮したモデル化 : 第 41 回複合材料シンポジウム 講演論文集, 2016
- 【5004 流体工学】
27. Abhishek L. Pillai, Masaya Muto, Ryoichi Kurose : Numerical investigation of effect of Reynolds number on noise from turbulent non-premixed hydrogen jet flames : In *Proc. of the Asian Congress on Gas Turbines (ACGT2016)*, pp.USB (9 pages) -, 2016
- 【5202 構造工学・地震工学・維持管理工学】
28. Kyohei Noguchi, Soichiro Hata, Hiromichi Shirato, Tomomi Yagi : Effect of de-icing salts scattered by vehicle running : *Proceedings of the Twenty-ninth KKHTCNN Symposium on Civil Engineering*, pp.525-528, 2016
29. 野口恭平, 秦聡一朗, 白土博通, 八木知己: 車両走行による凍結防止剤の飛散がもたらす周辺塩分環境の変化 : *土木学会第 71 回年次学術講演会講演概要集*, pp.91-92, 2016
- 【5401 金属物性】
30. S. Toyoda, K. Fukuda, K. Horiba, M. Oshima, K. Kumagai, Y. Kumagai, F. Oba, Y. Uchimoto, and E. Matsubara : Ligancy-driven controlling of covalency and metallicity in a ruthenium two-dimensional system : *Chem. Mater.*, Vol.28, pp.5784 - 5790, 2016
31. Y. Kumagai, L. A. Burton, A. Walsh, and F. Oba : Electronic structure and defect physics of tin sulfides: SnS, Sn<sub>2</sub>S<sub>3</sub>, and SnS<sub>2</sub> : *Phys. Rev. Applied*, Vol.6, pp.014009-1 - 014009-14, 2016
32. Y. Hinuma, T. Hatakeyama, Y. Kumagai, L. A. Burton, H. Sato, Y. Muraba, S. Iimura, H. Hiramatsu, I. Tanaka, H. Hosono, and F. Oba : Discovery of earth-abundant nitride semiconductors by computational screening and high-pressure synthesis : *Nature Commun.*, Vol.7, pp.11962-1 - 11962-10, 2016
33. Y. Hinuma, G. Pizzi, Y. Kumagai, F. Oba, and I. Tanaka : Band structure diagram paths based on crystallography : *Comput. Mater. Sci.*, Vol.128, No., pp.140 - 184, 2017
34. H. Hayashi, S. Katayama, T. Komura, Y. Hinuma, T. Yokoyama, K. Mibu, F. Oba, and I. Tanaka : Discovery of a novel Sn(II)-based oxide  $\beta$ -SnMoO<sub>4</sub> for daylight-driven photocatalysis : *Adv. Sci.*, Vol.4, pp.1600246-1 - 1600246-8, 2017
35. Y. Hinuma, Y. Kumagai, I. Tanaka, and F. Oba : Band alignment of semiconductors and insulators using dielectric-dependent hybrid functionals: Toward high-throughput evaluation : *Phys. Rev. B*, Vol.95, pp.075302-1 - 075302-10, 2017
36. Y. Kumagai, K. T. Butler, A. Walsh, and F. Oba : Theory of ionization potentials of nonmetallic solids : *Phys. Rev. B*, Vol.95, pp.125309-1 - 125309-10, 2017
- 【5403 複合材料・物性】
37. Shinya Iwata : Influence of Humidity Treatment on Electrical Tree Propagation in Epoxy Resin : *IEEE Transactions on Dielectrics and Electrical Insulation*, Vol.23, No.5, pp.2556-2561, 2016