

論文リスト List of papers

1. Just-In-Time Compiler System in Aspect-Oriented Programming based Building Block Platform for constructing Domain-Specific Language for HPC Application, O. Ishimura and Y. Yoshimoto, 2022 Tenth International Symposium on Computing and Networking Workshops, CANDARW 2022, pp. 241-247 (2022)
2. Aspect-Oriented Programming based building block platform to construct Domain-Specific Language for HPC application, Osamu Ishimura Yoshihide Yoshimoto, IEEE 36th International Parallel and Distributed Processing Symposium Workshops, IPDPSW 2022, pp. 457-466 (2022)
3. アスペクト指向言語を用いた HPC 向け DSL 作成プラットフォームにおけるメモリ管理手法の提案と評価, 石村 脩, 吉本 芳英, 情報処理学会研究報告, Vol. 2021-HPC-180, No.15 (2021)
4. *Ab initio* derivation of low-energy Hamiltonians for systems with strong spin-orbit interaction: Application to $\text{Ca}_5\text{Ir}_3\text{O}_{12}$, Maxime Charlebois, Jean-Baptiste Morée, Kazuma Nakamura, Yusuke Nomura, Terumasa Tadano, Yoshihide Yoshimoto, Youhei Yamaji, Takumi Hasegawa, Kazuyuki Matsuhira, and Masatoshi Imada, Phys. Rev. B Vol. 104, Art. No. 075153 (2021)
5. RESPACK: An ab initio tool for derivation of effective low-energy model of material, Kazuma Nakamura, Yoshihide Yoshimoto, Yusuke Nomura, Terumasa Tadano, Mitsuaki Kawamura, Taichi Kosugi, Kazuyoshi Yoshimi, Takahiro Misawa, and Yuichi Motoyama, Computer Physics Communications, Vol 261, Art. No. 107781 (2021)
6. Core-level shifts in x-ray photoelectron spectroscopy of arsenic defects in silicon crystal: A first-principles study, Jun Yamauchi, Yoshihide Yoshimoto, and Yuji Suwa, AIP Advances Vol. 10, Art. No. 115301 (2020)
7. Study of Phonon Dispersion of Iridium Oxide $\text{Ca}_5\text{Ir}_3\text{O}_{12}$ with Strong Spin Orbit Interaction, Hiroki Hanate, Takumi Hasegawa, Satoshi Tsutsui, Kazuma Nakamura, Yoshihide Yoshimoto, Naohiro Kishigami, Sho Haneta, and Kazuyuki Matsuhira, J. Phys. Soc. Jpn., Vol. 89, Art. No. 053601 (2020)
8. アスペクト指向言語を用いた HPC 向け DSL 作成プラットフォームの構築, 石村 脩, 吉本 芳英, 情報処理学会研究報告, Vol. 2019-HPC-170, No.42 (2019)
9. Formation of a two-dimensional single-component correlated electron system and band engineering in the nickelate superconductor NdNiO_2 , Yusuke Nomura, Motoaki Hirayama, Terumasa Tadano, Yoshihide Yoshimoto, Kazuma Nakamura, and Ryotaro Arita, Phys. Rev. B, Vol. 100, Art. No. 205138 (2019)
10. Self-ordering of chemisorbed PTCDA molecules on Ge(001) driven by repulsive forces, Pavel Kocin, Barbara Pieczykrak, Leszek Jurczyszyn, Yoshihide Yoshimoto, Kazuma Yagyu, Hiroshi Tochihara and Takayuki Suzuki, Physical Chemistry Chemical Physics, Vol. 21, 9504-9511 (2019)
11. ハードウェア階層構造を持つ HPC システム向けステンシル計算コードの自動最適化プラットフォームの提案と評価, 石村 脩, 吉本 芳英, 情報処理学会研究報告, Vol. 2018-HPC-165, No.35 (2018)

12. パフィアン計算の高速化, 今野 裕大, 吉本 芳英, 情報処理学会研究報告, Vol. 2018-ARC-231, No.3 (2018)
13. Nonlinear Conductivity of Geometrically Frustrated Iridate $\text{Ca}_5\text{Ir}_3\text{O}_{12}$, Kazuyuki Matsuhira, Kazuma Nakamura, Yuki Yasuskuni, Yoshihide Yoshimoto, Daigorou Hirai, and Zenji Hiroi, J. Phys. Soc. Jpn., Vol. 87, No. 1, Art. No. 013703 (2018)
14. Second order accuracy finite difference methods for space-fractional partial differential equations, Yuki Takeuchi, Yoshihide Yoshimoto, Reiji Suda, J. Comp. Appl. Math., Vol. 320, 101-119 (2017)
15. Adsorption of PTCDA on Ge(001), P. Kocan, Y. Yoshimoto, K. Yagyu, H. Tochihara, T. Suzuki, J. Phys. Chem. C., Vol. 121, 3320-3326 (2017)
16. HPC における HSA の性能評価, 石村 脩, 吉本 芳英, 情報処理学会研究報告, Vol. 2016-HPC-155, No.14 (2016)
17. X-ray photoelectron spectroscopy analysis of boron defects in silicon crystal: A first-principles study, Jun Yamauchi, Yoshihide Yoshimoto, Yuji Suwa, J. Appl. Phys., Vol. 119, Art. No. 175704 (2016)
18. Molecular dynamics and Monte Carlo hybrid simulation for fuzzy tungsten nanostructure formation, A. M. Ito, A. Takayama, Y. Oda, T. Tamura, R. Kobayashi, T. Hattori, S. Ogata, N. Ohno, S. Kajita, M. Yajima, Y. Noiri, Y. Yoshimoto, S. Saito, S. Takamura, T. Murashima, M. Miyamoto, H. Nakamura, Nuclear Fusion, Vol. 55, Art. No. 070313 (2015)
19. Hybrid simulation research on formation mechanism of tungsten nanostructure induced by helium plasma irradiation, Atsushi M. Ito, Arimichi Takayama, Yasuhiro Oda, Tomoyuki Tamura, Ryo Kobayashi, Tatsunori Hattori, Shuji Ogata, Noriyasu Ohno, Shin Kajita, Miyuki Yajima, Yasuyuki Noiri, Yoshihide Yoshimoto, Seiki Saito, Shuichi Takamura, Takahiro Murashima, Mitsutaka Miyamoto, Hiroaki Nakamura, J. Nucl. Mater., Vol. 463, 109-115 (2015) [NO refereeing]
20. Adsorption and self-assembled structures of sexithiophene on the $\text{Si}(111)-\sqrt{3} \times \sqrt{3}$ -Ag surface, Takashi Yokoyama, Mitsunori Kawasaki, Tomotaka Asari, Shinya Ohno, Masatoshi Tanaka and Yoshihide Yoshimoto, J. Chem. Phys. Vol. 142, Art. No. 204701 (2015)
21. Adsorption of PTCDA on $\text{Si}(001)-2 \times 1$ surface, Takayuki Suzuki, Yoshihide Yoshimoto, Kazuma Yagyu and Hiroshi Tochihara, J. Chem. Phys. Vol. 142, Art. No. 101904 (2015)
22. Molecular dynamics simulation of a helium bubble bursting on tungsten surfaces, Atsushi M Ito, Yoshihide Yoshimoto, Seiki Saito, Arimichi Takayama, Hiroaki Nakamura, Phys. Scr. Vol. T159, Art. No. 014062 (2014)
23. 第一原理計算の現状と課題を考える, 吉本芳英, 計算物質科学イニシアティブ newsletter Torrent No. 6, 6-7 (2012)
24. Ab initio two-dimensional multiband low-energy models of $\text{EtMe}_3\text{Sb}[\text{Pd}(\text{dmit})_2]_2$ and κ -(BEDT-TTF) $_2\text{Cu}(\text{NCS})_2$ with comparisons to single-band models, Kazuma Nakamura, Yoshihide Yoshimoto, and Masatoshi Imada, Phys. Rev. B, Vol. 86, Art. No. 205117 (2012)

25. Identification of boron clusters in silicon crystal by B1s core-level x-ray photoelectron spectroscopy: A first-principles study, Jun Yamauchi, Yoshihide Yoshimoto, and Yuji Suwa, Appl. Phys. Lett., Vol. 99, Art. No. 191901 (2011)
26. 第一原理電子状態計算と HPC, 吉本 芳英, 情報処理学会研究報告, Vol. 2010-HPC-125, No.4 (2010)
27. Ab initio Low-Dimensional Physics Opened Up by Dimensional Downfolding: Application to LaFeAsO, Kazuma Nakamura, Yoshihide Yoshimoto, Yoshiro Nohara, Masatoshi Imada, J. Phys. Soc. Jpn., Vol. 79, No. 12, p.123708 (2010)
28. Melting of MgO Studied Using a Multicanonical Ensemble Method, Yoshihide Yoshimoto, J. Phys. Soc. Jpn., Vol. 79, No. 3, p.034602 (2010)
29. *Ab initio* Derivation of Low-Energy Model for κ -ET Type Organic Conductors, Kazuma Nakamura, Yoshihide Yoshimoto, Taichi Kosugi, Ryotaro Arita, Masatoshi Imada, J. Phys. Soc. Jpn., Vol. 78, No. 8, p. 083710 (2009)
30. Dissociative Adsorption of Oxygen on Clean Cu(001) Surface, Kazuma Yagyu, Xiangdong Liu, Yoshihide Yoshimoto, Kan Nakatsuji and Fumio Komori, J. Phys. Chem. C, Vol. 113, No. 14, pp. 5541-5546 (2009)
31. Model potential of dimer system and coherence length of electron injected by scanning tunneling microscope on Ge(001) surface, H. Kawai, Y. Yoshimoto, O. Narikiyo, Y. Hanawa, A. Imamura, Surf. Sci. Vol. 602, No. 18, pp. 3010-3017 (2008)
32. Electron correlation effects in Co nanoscale islands on a nitrogen-covered Cu(001) surface, K. Nakatsuji, Y. Yoshimoto, D. Sekiba, S. Doi, T. Iimori, K. Yagyu, Y. Takagi, S. Ohno, H. Miyaoka, M. Yamada, F. Komori, K. Amemiya, D. Matsumura, and T. Ohta, Phys. Rev. B Vol. 77, No. 23, Art. No. 235436 (2008)
33. Optical absorption study by ab initio downfolding approach: Application to GaAs, K. Nakamura, Y. Yoshimoto, R. Arita, S. Tsuneyuki, M. Imada, Phys. Rev. B Vol 77, No. 19, Art. No. 195126 (2008)
34. Nanopattern formation on Cu(001) surface coadsorbed with nitrogen and oxygen, K. Yagyu, K. Nakatsuji, Y. Yoshimoto, S. Tsuneyuki, and F. Komori, Surf. Sci. Vol. 601, No. 21, pp. 4837-4842 (2007)
35. Superstructure manipulation on a clean Ge(001) surface by carrier injection using an STM, Y. Takagi, K. Nakatsuji, Y. Yoshimoto, F. Komori, Phys. Rev. B, Vol. 75, No. 11, Art. No. 115304 (2007)
36. Strain-induced change in electronic structure of Cu(100), D. Sekiba, Y. Yoshimoto, K. Nakatsuji, Y. Takagi, T. Iimori, S. Doi, F. Komori, Phys. Rev. B, Vol. 75, No. 11, Art. No. 115404 (2007)
37. Effect of encapsulated atoms on the electronic structure of the fullerene cage: A case study on La-2@C-78 and Ti2C2@C-78 via ultraviolet photoelectron spectroscopy, S. Hino, M. Kato, D. Yoshimura, H. Moribe, H. Umemoto, Y. Ito, T. Sugai, H. Shinohara, M. Otani, Y. Yoshimoto, S. Okada, Phys. Rev. B, Vol. 75, No. 12, Art. No. 125418 (2007)

38. 第一原理計算による構造最適化とその周辺, 吉本 芳英, 表面科学, Vol. 28, No. 3, pp. 144-149 (2007)
39. First-principles calculation of effective onsite Coulomb interactions of 3d transition metals: Constrained local density functional approach with maximally localized Wannier functions, K. Nakamura, R. Arita, Y. Yoshimoto, S. Tsuneyuki, Phys. Rev. B, Vol. 74, No. 23, Art. No. 235113 (2006)
40. Formation of dihydride chains on H-terminated Si(100)- 2×1 surfaces: Scanning tunneling microscopy and first-principles calculations, Y. Suwa, M. Fujimori, S. Heike, Y. Terada, Y. Yoshimoto, K. Akagi, O. Sugino, T. Hashizume, Phys. Rev. B, Vol. 74, No. 20, Art. No. 205308 (2006)
41. Extended multiccanonical method combined with thermodynamically optimized potential: application to the liquid-crystal transition of silicon, Y. Yoshimoto, J. Chem. Phys., Vol. 125, No. 18, Art. No. 184103 (2006)
42. First principles study of dihydride chains on H-terminated Si(100)- 2×1 surface, Y. Suwa, M. Fujimori, S. Heike, Y. Terada, Y. Yoshimoto, K. Akagi, O. Sugino, T. Hashizume, Jpn. J. Appl. Phys., Vol. 45, No. 3B, pp. 2200-2203 (2006)
43. Nonlocal manipulation of dimer motion at Ge(001) clean surface via hot carriers in surface states, Y. Takagi, Y. Yoshimoto, K. Nakatsuji, F. Komori, J. Phys. Soc. Jpn., Vol 74, No. 12, pp. 3143-3146 (2005)
44. Role of a topological defect in the local structure transformation on clean Ge(001) surface by STM, Y. Takagi, Y. Yoshimoto, K. Nakatsuji, F. Komori, Surf. Sci., Vol. 593, No. 1-3, pp. 133-138 (2005)
45. Direct observation of strain-induced change in surface electronic structure, D. Sekiba, K. Nakatsuji, Y. Yoshimoto, F. Komori, Phys. Rev. Lett., Vol. 94, No. 1, Art. No. 016808 (2005)
46. Nanotube-based molecular magnets with spin-polarized edge states, Y. Higuchi, K. Kusakabe, N. Suzuki, S. Tsuneyuki, J. Yamauchi, K. Akagi, Y. Yoshimoto, J. Phys.: Condens. Matter, Vol 16, No 48, pp. S5689-S5692 (2004)
47. First-principles study on the strain effect of the Cu(001)- $c(2 \times 2)$ self-organized structure, Y. Yoshimoto and S. Tsuneyuki, Appl. Surf. Sci., Vol. 237, No. 1-4, pp. 274-278 (2004)
48. Reversible local-modification of surface structure on clean Ge(001) by scanning tunneling microscopy below 80 K, Y. Takagi, Y. Yoshimoto, K. Nakatsuji and F. Komori, Surf. Sci., Vol. 559, No. 1, pp. 1-15 (2004)
49. Molecular scale structure formation by folding, Y. Yoshimoto, Surf. Sci., Vol. 556, No. 1, pp. 52-62 (2004)
50. Magnetic properties of nanographite with modified zigzag edges, M. Maruyama, K. Kusakabe, S. Tsuneyuki, K. Akagi, Y. Yoshimoto and J. Yamauchi, J. Phys. Chem. Solids, Vol. 65, No. 2-3, pp. 119-122 (2004)
51. Local and Reversible Change of the Reconstruction on Ge(001) Surface between $c(4 \times 2)$ and $p(2 \times 2)$ by Scanning Tunneling Microscopy, Y. Takagi, Y. Yoshimoto, K. Nakatsuji and F. Komori, J. Phys. Soc. Jpn., Vol. 72, No. 10, pp. 2425-2428 (2003)

52. Data fitting with a spline using a real-coded genetic algorithm, Fujiichi Yoshimoto, Toshinobu Harada, Yoshihide Yoshimoto, *Computer-Aided Design*, Vol.35, No. 8, pp. 751-760 (2003)
53. First-principles study of inter nitrogen interaction energy of Cu(100)- $c(2 \times 2)$ N surface, Y. Yoshimoto and S. Tsuneyuki, *Int. J. Quant. Chem.*, Vol. 91, No. 2, pp. 211-215 (2003)
54. Model Potential for the Dimer System on the Si(001) Surface Improved by a First-Principles Calculation and Structural Fluctuation Studied by a Monte Carlo Simulation, H. Kawai, R. Miyata, Y. Yoshimoto, and M. Tsukada, *J. Phys. Soc. Jpn.*, Vol. 72, No. 12, pp. 3158-3163 (2003)
55. First-principles study of inter nitrogen interaction energy of Cu(100)- $c(2 \times 2)$ N surface, Y. Yoshimoto and S. Tsuneyuki, *Surf. Sci.*, Vol. 514, No. 1-3, pp. 200-205 (2002)
56. Time-Fluctuation of the Dimer Structure on a Ge(001) Surface Studied by a Monte Carlo Simulation and a First-Principles Calculation, H. Kawai, Y. Yoshimoto, H. Shima, Y. Nakamura and M. Tsukada *J. Phys. Soc. Jpn.*, Vol. 71, No. 9, pp. 2192-2199 (2002)
57. Monte Carlo simulation of temperature dependence of X-ray diffraction intensity of Ge(001) surface with defects, Y. Nakamura, H. Kawai, Y. Yoshimoto, M. Tsukada, *Surf. Sci.*, Vol. 493 No. 1-3, pp. 361-365 (2001)
58. 実数を遺伝子とした遺伝的アルゴリズムによるデータあてはめ, 吉本富士市, 原田利宣, 森山真光, 吉本芳英情報処理学会論文誌, Vol. 41, No. 1, pp. 70-82 (2000)
59. Ge(001) surface reconstruction studied using a first-principles calculation and a Monte Carlo simulation, Y. Yoshimoto, Y. Nakamura, H. Kawai, M. Tsukada, and M. Nakayama, *Phys. Rev. B*, Vol. 61, No. 3, pp. 1965-1970 (2000)
60. The Ge(001) Surface Reconstruction: DFT and MCS, Y. Yoshimoto, Y. Nakamura, H. Kawai, M. Tsukada, and M. Nakayama, *Surface Review and Letters*, Vol. 6, No. 6, pp. 1045-1051 (1999)
61. First principles study on the geometry and stability of the Ge atom in initial Ge growth on the Si(001) surface, Y. Yoshimoto and M. Tsukada, *Surf. Sci.*, Vol. 423, No. 1, pp. 32-42 (1999)
62. Methanol traps the Troponin-Tropomyosin-actin complex in an off-state, Y. Matsuura, Y. Yoshimoto, K. Saeki, T. Wakabayashi, *J. Biochem.*, Vol. 118, No. 6, pp. 1293-1296 (1995)