

Publication List

Atsushi Oshiyama

(A) Original Papers

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(B) Review Papers and Books

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(C) Invited Talks

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4. 押山淳, “Understanding and Finding of Phenomena Related to Design of New Materials”, 日本物理学会 (広島大学, 1988).
5. 押山淳, “Mechanisms of Self-Diffusion in Silicon” 日本物理学会 (大阪大学, 1990).
6. A. Oshiyama, “Microscopic Theory of Oxidation of Si and Formation of Si/SiO₂ Interface”, *Int. Workshop on Computational Materials Science*, Tsukuba (1990).
7. 斎藤晋, 押山淳, “Electron States of C₆₀”, 日本物理学会 (北海道大学, 1991).
8. 斎藤晋, 押山淳, “Electronic Structure and Superconductivity of Alkali-doped C₆₀”, 日本物理学会 (北海道大学, 1991).
9. A. Oshiyama, “Atomic Structure, Electron States and Superconductivity of C₆₀ Fullerides”, *Sympo. Theoretical Solid State Physics* (Korea, 1992).

10. A. Oshiyama, Y. Miyamoto and M. Hane, "Microscopic Calculation for the Initial Stage of Silicon Oxidation", International Workshop on Science and Technology for Surface reaction Process (Takehashi, Tokyo, 1992).
11. 押山淳, "Microscopic Mechanisms of Atomic Diffusion in Si under Pressure", 日本物理学会 (慶應大学, 1992).
12. 押山淳, "Mechanisms and Control of Impurity Diffusion in Si", 応用物理学会学術講演会 (日本大学, 1992).
13. 押山淳, "Microscopic Theory of Initial Stage of Silicon Oxidation", 応用物理学会学術講演会 (日本大学, 1992).
14. S. Saito and A. Oshiyama, "Electronic Structure and Superconductivity of Fullerenes and Fullerides", *181st Electrochemical Society Meeting* (St Louise, 1992).
15. A. Oshiyama, "Electronic Structure of C₆₀ and Related Materials", *US/Japan Seminar on Electronic Structure and Fermiology of High T_c Superconductors* (Sendai, 1992).
16. (**Plenary**) S. Saito, A. Oshiyama, Y. Miyamoto, N. Hamada and S. Sawada, "Cohesion, Electron States and Superconductivity of Fullerenes and Fullerides", *21st Int. Conf. Physics of Semiconductors* (Beijing, 1992).
17. N. Hamada, S. Sawada and A. Oshiyama, "Carbon Nanotubes: Electronic Structure", *MRS Fall Meeting* (Boston, 1992).
18. A. Oshiyama, "Ab-initio Approach to Atomic and Electronic Structures of Materials: From C₆₀ to Silicon", *2nd Int. Conf. on Computer Applications to Materials and Molecular Science and Engineering (CAMSE)* (September 1992, Yokohama).
19. (**Plenary**) A. Oshiyama, "Electronic Structure and Superconductivity of C₆₀ Fullerides", *5th Asia-Pacific Physics Conference* (Kuala Lumpur, August 1992).
20. A. Oshiyama, "C₆₀ as a Superatom: Electronic Structure of Doped Fullerides", *182nd Electrochemical Society Meeting* (Tronto, 1992).
21. A. Oshiyama, "Conjugate-Gradient Total-Energy Minimization: Defects in Silicon", *15th Taniguchi Symp. on Interatomic Potential and Structural Stability* (Shima, 1993).
22. Y. Miyamoto, A. Oshiyama, N. Hamada, and S. Saito, "Electronic Structure of Doped Solid C₆₀" *TMS Conference* (Denver, 1993).
23. A. Oshiyama, "Total-Energy Electronic-Structure Calculations: From Si to Carbon 60" *6th Brazilian School on Semiconductor Physics* (Sao Carlos, July 1993).
24. A. Oshiyama, "Covalency, Elasticity and Electron Correlation in Si Vacancies" *6th Int. Workshop on Slow-Positron Beam Technology for Solids and Surfaces* (Makuhari, Japan 1994).

25. 押山淳, “Structures of Steps and Appearance of facets on Si(100)”, 応用物理学会学術講演会 (名城大学, 1994).
26. 押山淳, “Theory of Atomic Reactions on Semiconductor Surfaces”, 日本物理学会第51回年会 (金沢大学, 1996).
27. 押山淳, “As a Theorist” 日本物理学会第51回年会格子欠陥分科シンポジウム (金沢大学, 1996).
28. A. Oshiyama, “Microscopic Surface Structures and Macroscopic Thin-Film Morphology in Semiconductor Epitaxial Growth” *8-th International Conference on Solid Films and Surfaces* (Osaka, Japan; July, 1996).
29. A. Oshiyama, “LDA Approach to Understanding of Mechanisms of Semiconductor Epitaxial Growth” *2'nd International Symposium on Controle of Semiconductor Interfaces* (Karuizawa, Japan; October, 1996).
30. 押山淳, “Bistability of Oxygen Vacancy in SiO₂ and its degradation” 日本物理学会 (神戸大学, 1997).
31. A. Oshiyama, “First Principles Calculations on Vacancies in Silicon” Proc. *Kazusa Akademia Park Forum on Science and Technology of Silicon Materials* (Chiba, November 1997).
32. A. Oshiyama, “Complex Diffusion Mechanisms of Si Adatom on Hydrogenated Si(100)” Int. Workshop on Large-Scale Quantum Simulations: Total Energy and Force Methods” (Tsukuba, January 1998).
33. A. Oshiyama, “Density-Functional Calculations for Semiconductor Epitaxial Growth and for Defects in Materials” APCTP/ICTP Joint International Conference on Highlights in Condensed Matter Physics (Seoul, June 1998).
34. A. Oshiyama, “Do First-Principles Calculations Work in Development of Materials” 17'th Electronic Materials Symposium (Sizuoka, July 1998).
35. 押山淳, “Hydrogen in Si Epitaxial Growth: Energetics and Kinetics” 応用物理学会第59回学術講演会 (広島大学, 1998).
36. 押山淳, “Hydrogenated Si Surfaces: Diffusion and Dynamics” 日本物理学会 (琉球大学, 1998).
37. A. Oshiyama, “Mechanisms of Semiconductor Epitaxial Growth: Approach from the First-Principles Calculations” NCCG-30 (Japanese Association for Crystal Growth), (Fukuoka, Japan, 1999).
38. J. Jeong and A. Oshiyama, “Microscopic Mechanisms of B Diffusion in Si” 2'nd Korean-Japan Joint Workshop on Electronic Structure Calculations (Seoul, 1999).

39. A. Oshiyama, “Ga Wires on Si(100) Surfaces: Possible Ferromagnets on Semiconductors” 5th Symposium on the Physics and Application of Spin-related Phenomena in Semiconductors (Sendai, Japan, 1999).
40. S. Jeong and A. Oshiyama, “Mechanisms of Epitaxial Growth on Si(100) Surfaces” 8-th Asia Pacific Physics Conference, (Taipei, 2000).
41. (**plenary**) A. Oshiyama, “First-Principles Calculations for Mechanisms of Semiconductor Epitaxial Growth” 13-th Int. Conf. on Crystal Growth (Kyoto, 2001)
42. A. Oshiyama, “Prediction of Electronic Properties of Carbon-Based Nanostructures” Tsukuba Symposium on Carbon Nanotube (Tsukuba, October 2001).
43. A. Oshiyama, “Prediction of Electronic Properties of Carbon-Based Nanomaterials” International Workshop on Materials Simulation (Shonan, Japan, November 2001).
44. 押山淳, “炭素ベースナノ構造の新物性：ピーポッドとフレーク” 第22回フラレン総合シンポジウム (岡崎、2002年1月) .
45. A. Oshiyama, “New Properties of Carbon-Based Nanostructures: Tubes, Peapods and Flakes” 16th International Winterschool on Electronic Properties of Novel Materials (Kirchberg/Tirol, Austria, March 2002).
46. A. Oshiyama, “Prediction of New Properties of Nanoscale Materials” FIMS/ITNs-2003 (2nd International Symposium on Future-Oriented Interdisciplinary Materials Science / 1st International Tsukuba Symposium on Nanoscience) (Tsukuba, November 2003).
47. A. Oshiyama, “Density Functional Approach to Hard and Soft Nanomaterials” ICTP Asian/Pacific Regional School on *Electronic Structure Methods and Their Applications* (Beijin, July 2004).
48. 押山淳, “Behavior of Oxygen Atoms and Bond Formation in SiO₂: Free Energy Molecular Dynamics Approach” 日本物理学会 (青森大学, 2004).
49. A. Oshiyama, “Nano-shapes and Electronic Properties of Carbon Materials” 12th International Workshop on Computational Physics and Materials Science: Total Energy and Force Methods (ICTP, Trieste, Italy; January, 2005)
50. M. Boero, A. Oshiyama, P. L. Silvestrelli and K. Murakami, “First-principle molecular dynamics study of bond disruption and formation in SiO₂ upon irradiation”, 23rd Int. Conf. Defects in Semiconductors (Awaji, July, 2005).
51. 押山淳, 「SiO₂ へのレーザー照射効果」 日本物理学会秋季大会シンポジウム「電子励起と不純物ダイナミクスのコントロール」(2005年9月、同志社大学)
52. 押山淳, 「ナノ・バイオ物質における密度汎関数法計算」 計算科学の基盤技術とその発展：RIMS 研究集会 (2005年12月、京都大学)

53. 押山淳, 「ナノ・バイオ物質での密度汎関数法計算: 現象の微視的機構と予測」 ナノ学会第4回大会 (2006年5月, 京都大学)
54. A. Oshiyama, “Prediction of Atomic and Electronic Structures of Hybrid Materials with Carbon Nanotubes” International Workshop on Computational Challenges and Tools for Nanotubes (Nagano, June, 2006)
55. A. Oshiyama, “Atomic and Electronic Structures of Carbon nanotubes on Si and Metal Surfaces” 9th Asian Workshop on First-Principles Electronic-Structure Calculations (Seoul, November, 2006).
56. A. Oshiyama, “Carbon Nanotube and its Hybrid Structures” 2nd Int. Symposium on Nanometer-Scale Quantum Physics (nanoPHYS07), (Tokyo, January 24-26, 2007)
57. 押山淳, “密度汎関数理論によるナノ・バイオ計算”, Supercomputer Workshop 2007 計算分子科学の30年と将来、(自然科学研究機構, 2007年2月)
58. 押山淳, “Current Stage of the Density Functional Approach Toward Atom Dynamics upon electron Excitation” 日本物理学会 2007年春季大会シンポジウム「Atom Dynamics and Formation of Nano-objects by Electronic Excitation」(2007年3月、鹿児島大学)
59. A. Oshiyama, “Proton Transfer in Cytochrome c Oxidase using CPMD + Metadynamics” Roberto Car 60th Birthday Symposium (Trieste, June 21-23, 2007)
60. A. Oshiyama, “Density-Functional Approach to Nano- and Bio-Materials” ICYS(NIMS)-ICMR(UC Santa Barbara) Summer School on Nanomaterials (Tsukuba, July 23-28, 2007)
61. A. Oshiyama, “Microscopic Mechanisms of Proton Transfer in Cytochrome c Oxidase: Car-Parrinello Metadynamics Approach” Handai Nanoscience and Nanotechnology International Symposium (Osaka, September 26-28, 2007)
62. A. Oshiyama, “Large-scale Density-Functional Calculations using Real-Space Parallel-Computation Technique”, 1st Int. Conf. of The Grand Challenge to Next-Generation Integrated Nanoscience (June 3 - 7, 2008, Tokyo)
63. Y. Fujimoto, T. Korestune, S. Saito, T. Miyake, and A. Oshiyama, “Structural and electronic properties of new crystalline phase of Si and Ge”, International Conference on Quantum Simulators and Design, (2008/6/2, Tokyo)
64. A. Oshiyama “Cation Vacancies in Nitride Semiconductors: A Possibility of Intrinsic Ferromagnetism”, JST-DFG Workshop on Nanoelectronics, (January 21-23, 2009, Kyoto).
65. A. Oshiyama, “Real-Space Density-Functional-Theory Scheme and its Application to Large Systems”, Supercomputing in Solid State Physics, (February 16 -19, 2009, Kashiwa, Chiba).

66. 押山淳, “ナノ構造体の面白さ - 電子論による機能探索” 第 56 会応用物理学関係連合講演会シンポジウム「ポストスケール時代をデバイス・物性物理から斬る - これが半導体デバイスの未来像だー」(2009 年 3 月、筑波大学)
67. A. Oshiyama, “Intrinsic Ferromagnetism due to cation Vacancies in Nitride Semiconductors”, Scientific Symposium Honoring Sok Pantelides - Recent Advances in Materials Physics, (April 3 - 5, Vanderbilt University, USA)
68. A. Oshiyama, “Large-Scale Density-Functional Calculations for Atomic and Electronic Structures of Si Nanowires” PICE International Symposium on Silicon Nano Devices in 2030: Prospects by World’s Leading Scientists (October 13-14, 2009, Tokyo, Japan).
69. A. Oshiyama, “Large-Scale Density Functional Calculations for Silicon and Carbon Nanostructures”, Conference on Computational Physics 2009 (Kaoshing, Taiwan, December 15 - 19, 2009)
70. A. Oshiyama, “Large-Scale Density Functional Calculations in Real Space Scheme”, Int. Workshop on Computational Physics and Materials Sciences: total energy and force method (Shanghai, January 7 - 9, 2010)
71. A. Oshiyama, “Current Status of Density-Functional-Theory-Based Calculations for Nano- and Bio-Materials”, Int. Sympo. “Nanoscience and Quantum Physics 2011” (Tokyo, January 26-28, 2011).
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