

# Publications and Invited Talks

Atsushi Oshiyama

## (A) Original Papers

1. Y. Fujimoto and A. Oshiyama, “Structural Stability and Scanning Tunneling Microscopy Images of Strained Ge Films on Si(001)” *Phys. Rev. B* **87**, 075323 (2013).
2. S. Kyogoku, J.-I. Iwata and A. Oshiyama, “Relation between nanomorphology and energy bands of Si nanowires” *Phys. Rev. B* **87**, 165418 (2013).
3. K. Uchida and A. Oshiyama, “New identification of Metallic Phases of In Atomic layers on Si(111) Surfaces” *Phys. Rev. B* **87**, 165433(2013). DOI: 10.1103/PhysRevB.87.165433
4. K. Koizumi, M. Boero, Y. Shigeta, and A. Oshiyama, “Atom-Scale Reaction Pathways and Free-Energy Landscapes in Oxygen Plasma Etching of Graphene” *J. Phys. Chem. Letters* **4**, 1592 (2013).
5. Z.-X. Guo, S. Furuya, J.-I. Iwata and A. Oshiyama, “Absence of Dirac Electrons in Silicene on Ag(111) Surfaces” *J. Phys. Soc. Jpn. Letters* **82**, 063714 (2013).
6. E. K. K. Abavare, J.-I. Iwata and A. Oshiyama, “Atomic Reconstruction and Electron States at Interfaces between 3C-SiC(111) and Si(110)” *Phys. Rev. B* **87**, 235321 (2013). DOI: 10.1103/PhysRevB.87.235321
7. Z.-X. Guo, S. Furuya, J.-I. Iwata and A. Oshiyama, “Absence and Presence of Dirac Electrons in Silicene on Substrates” *Phys. Rev. B* **87**, 235435 (2013). DOI: 10.1103/PhysRevB.87.235435
8. Y. Hasegawa, J.-I. Iwata, M. Tsuji, D. Takahashi, A. Oshiyama, K. Minami, T. Boku, H. Inoue, Y. Kitazawa, I. Miyoshi, M. Yokokawa, “Performance evaluation of ultra-largescale first-principles electronic structure calculation code on the K computer” *Int. J. HPC Applications* (2013).
9. K. Sawada, J.-I. Iwata and A. Oshiyama, “First-Principles Study of Nanofacet Formation on 4H-SiC(0001) Surface” *Proc. Int. Conf. Silicon Carbide and Related Materials (ICSCRM)* (2013).
10. K. Uchida, Z.-X. Guo, J.-I. Iwata and A. Oshiyama, “Large-Scale Electronic-Structure Calculations in the Real-Space Scheme: Bilayer Graphene and Silicene” *Proc. JSAP-MRS Joint Symposia* (2013).

## (B) Review and Books

1. 押山淳, “結晶性半導体エピタキシャル成長の量子論” ポストシリコン半導体：ナノ成膜ダイナミクスと基板・界面効果, (エヌ・ティー・エス、2013) pp32 - pp42.

(C) Invited Talks

1. A. Oshiyama, “Materials Design through Computics: Large-Scale Density-Functional Calculations for Nanomaterials in the Real-Space Scheme” Int. Summer School on HPC Challenges in Computational Sciences (New York City, USA, June 2013).
2. A. Oshiyama, “Large-Scale Density-Functional Calculations in the Real-Space Scheme: Graphene and Silicene” 7th Conf. Asian Consortium on Computational Materials Science (ACCMS7) (Nakhon Ratchasima, Thailand, July 2013).
3. Z.-X. Guo, J.-I. Iwata and A. Oshiyama “Large-Scale Calculations in the Real-Space Scheme: Absence and Presence of Dirac Electrons in Silicene” 22th Int. Materials Research Congress (IMRC) 2013 (Cancun, Mexico, August, 2013)
4. A. Oshiyama “Large-Scale Electronic-Structure Calculations in the Real-Space Scheme: Bilayer Graphene and Silicene” 2013 JSAP-MRS Joint Symposia (Kyoto, September, 2013).