

Publications and Invited Talks

Atsushi Oshiyama

(A) Original Papers

1. 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” *International Journal High Performance Computing Applications*, **28**, 335-355 (2014). online version Oct 17, 508163 (2013). DOI=10.1177/1094342013508163
2. B. Enkhtaivan, M. Yoshimura, J.-I. Iwata, and A. Oshiyama, “Diameter-Selective Alignment of Carbon Nanotubes on Si(001) Stepped Surfaces” *J. Chem. Phys.* **140**, 044713 (2014).
3. K. Sawada, J.-I. Iwata and A. Oshiyama “Magic Angle and Height Quantization in Nanofacets on SiC(0001) Surfaces”, *Appl. Phys. Lett.* **104**, 051605 (2014).
4. Y. Matsushita and A. Oshiyama, “Interstitial Channels that Control Band Gaps and Effective Masses in Tetrahedrally Bonded Semiconductors”, *Phys. Rev. Lett.* **112**, 136403 (2014).
5. Z.-X. Guo and A. Oshiyama “Structural Tristability and Deep Dirac States in Bilayer Silicene on Ag(111) Surfaces”, *Phys. Rev. B* **89**, 155418 (2014).
6. E. K. K. Abavare, I.-I. Iwata, A. Yaya and A. Oshiyama, “Surface energy of Si(110)- and 3C-SiC(111)-terminated surfaces”, *Phys. Status Solidi B* **251**, 1408 - 1415 (2014) DOI 10.1002/pssb201350335.
7. Y.-i. Matsushita S. Furuya, and A. Oshiyama, “Electron Confinement due to Stacking Control of Atomic Layers in SiC Polytypes: Role of Floating States and Spontaneous Polarization” *J. Phys. Soc. Jpn.* **83**, 094713 (2014).
8. K. Uchida, S. Furuya, J.-I. Iwata and A. Oshiyama, “Atomic corrugation and electron localization due to Moiré patterns in twisted bilayer graphenes” *Phys. Rev. B* **90**, 155451 (2014).

(C) Invited Talks

1. A. Oshiyama, “Large-Scale Real-Space Density-Functional Calculations: Moiré-Induced Electron Localization in Graphene and Floating States in SiC” 32nd International Conference on the Physics of Semiconductors (Austin, Texas, USA, August 2014).