Publications and Invited Talks

Atsushi Oshiyama

(A) Original Papers

1. B. Enkhtaivan and A. Oshiyama, "Atomic Force Microscope manipulation of Ag atom on the Si(111) surface" Phys. Rev. B **95**, 035309 (2017).

2. H. Nishi, Y-i. Matsushita, A. Oshiyama, "Band-unfolding approach to moiré-induced band-gap opening and Fermi-level-velocity reduction in twisted bilayer graphene" Phys. Rev. B (2017) **95**, 085420 (2017).

3. H. Li, Y.-i. Matsushita, M. Boero and A. Oshiyama, "First-Principles Calculations that Clarify Energetics and Reactions of Oxygen Adsorption and Carbon Desorption on 4H-SiC ($11\bar{2}0$) Surface", J. Phys. Chem. C **121**, 3920 - 3928 (2017).

4. F. Imoto, J.-I. Iwata, M. Boero, A. Oshiyama, "Microscopic Mechanisms of Initial Formation Process of Graphene on SiC(0001) Surfaces: Selective Si Desorption from Step Edges" J. Phys. Chem. C **121**, 5041 - 5049 (2017).

5. Y.-i. Matsushita1 and A. Oshiyama, "Comprehensive study on band-gap variations in sp^3-bonded semiconductors: roles of electronic states floating in internal space" J. Phys. Soc. Jpn **86**, 054702 (2017).

6. B. Enkhtaivan, Y. Sugimoto and A. Oshiyama,"First-principles study of lateral atom manipulation assisted by structural relaxation of a scanning tip apex" Phys. Rev. B **96**, 155417 (2017). October 6

7. Y.-i. Matsushita and A. Oshiyama, "A novel intrinsic interface state controlled by atomic stacking sequence at interface of SiC/SiO_2" Nano Lett. **17**, 6458-6463 (2017). September 12

8. J.-I. Iwata, Y.-i. Matsushita, H. Nishi, Z.-X. Guo, and A. Oshiyama, "Mining single-electron spectra of the interface states from a supercell band structure of silicene on an Ag(111) substrate with band-unfolding methodology" Phys. Rev B **96**,235442 (2017). December 29

9. Y.-i. Matsushita, H. Nishi, J.-i. Iwata, T. Kosugi and A. Oshiyama, "Unfolding energy spectra of double-periodicity two dimensional systems: twisted bilayer graphene and MoS_2 on graphene" Phys. Rev. Materials **2**, 010801 (R) (2018). January 25

10. Y.-i. Matsushita and A. Oshiyama, "Mechanisms of initial oxidation of 4H-SiC (0001) and ($000\bar{1}$) surfaces unraveled by first-principles calculations" arXiv:1612.00189

(C) Invited Talks

1. A. Oshiyama, "Large-Scale Static and Dynamic Density-Functional Calculations in a Real-Space Scheme: New Physical Properties of Two-Dimensional Systems" The Platform for Advanced Scientific Computing Conference (PASC17), (June 25 - 28, 2017, Lugano, Switzerland)