

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. Matsushita 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” to appear in *Phys. Rev. B* (2017).
7. 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
8. Y.-i. Matsushita, H. Nishi, J.-i. Iwata, T. Kosugi and A. Oshiyama, “Unfolding energy spectra of multi-periodicity materials” arXiv:1706.05921
9. Y.-i. Matsushita and A. Oshiyama, “A novel intrinsic interface state controlled by atomic stacking sequence at interface of SiC/SiO $_2$ ” arXiv:1704.07094

(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)