

# Publications and Invited Talks

Atsushi Oshiyama

## (A) Awards

1. ACM Gordon Bell Prize 2011 (Peak Performance) *First-Principles Calculation of Electronic States of a Silicon Nanowire with 100,000 Atoms on the K Computer*

## (B) Original Papers

1. H. Iwai, K. Natori, K. Shiraishi, J.-I. Iwata, A. Oshiyama, K. Yamada, K. Ohmori, K. Kakushima and P. Ahmet, “Si Nanowire FET and Its Modeling” *Science China* **54**, 1004 - 1011 (2011).
2. Y. Matsushita, K. Nakamura and A. Oshiyama, “Comparative study of hybrid functionals applied to structural and electronic properties of semiconductors and insulators” *Phys. Rev. B* **84**, 075205 (2011).
3. A. Oshiyama and J.-I. Iwata, “Large-scale electronic-structure calculations for nanomaterials in density functional theory” *J. Phys: Conference Series* **302**, 012030 (2011).
4. S. Jeong and A. Oshiyama, “Selective Alignment of Carbon Nanotubes on Sapphire Surfaces: Bond Formation between Nanotubes and Substrates” *Phys. Rev. Lett.* **107**, 065501 (2011).
5. S. Kyogoku, J.-I. Iwata, and A. Oshiyama, “First-principle Study of Energy-Band Control by Cross-Sectional Morphology in [110]-Si Nano Wires” *Proc. IEEE Int. Conf. Nanotechnology (Portland, August 2011)* pp1322-1326.
6. Y. Hasegawa, J.-I. Iwata, M. Tsuji, D. Takahashi, A. Oshiyama, K. Minami, T. Boku, F. Shoji, A. Uno, M. Kurokawa, H. Inoue, I. Miyoshi, M. Yokokawa, “First-principles calculations of electron states of a silicon nanowire with 100,000 atoms on the K computer”, *Proceedings of 2011 International Conference for High Performance Computing, Networking, Storage and Analysis (SC2011)*
7. K. Koizumi, M. Boero, Y. Shigeta and A. Oshiyama, “Self-diffusion in crystalline silicon: Car-Parrinello molecular dynamics study”, *Phys. Rev B* **84**, 205203:1-10 (2011).

## (C) Review and Books

1. 合田義弘, 押山淳, 常行真司, “磁性元素が関与しない磁性? 界面・点欠陥の役割を予測” 日本物理学会誌, **66**, 836 (2011).

(D) Invited Talks

1. 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).
2. 押山淳, “励起ナノプロセス入門 - 第一原理計算” 第48回応用物理学会スクール(2011年8月29日、山形大学)
3. 押山淳, “PACS-CSにおける物性物理学研究” 第2回「学際計算科学による新たな知の発見・統合・創出」シンポジウム (2011年9月1日、筑波大学)
4. 押山淳, “コンピューティクスによる物質デザイン: RSDFTを例として” 東京大学物性研究所計算物質科学研究センター第1回シンポジウム (2011年9月12-13日、東京大学)
5. A. Oshiyama, “Materials Design through Computics: nanowires and Nanotubes” International Focus Workshop on Quantum Simulations and Design (September 27, 2011, Dresden, Germany)