

誌 上 発 表 **Publications**

[雑誌]

(原著論文) *印は査読制度がある論文誌

- Fujisaki H., Yagi K., Straub J. E., and Stock G.: “Quantum and classical vibrational relaxation dynamics of N-methylacetamide on ab initio potential energy surfaces”, *Int. J. Quantum Chem.* **109**, No. 10, pp. 2047–2057 (2009). *
- Ogawa T., Kawasaki Y., Takizawa Y., Ebisuzaki T., Sakaki N., Higuchi M., Uchihori Y., Kitamura H., and Wada S.: “Radiation Resistance of Nd-Doped Laser Crystals for Space Application”, *Jpn. J. Appl. Phys.* **48**, 088001-1–088001-2 (2009). *
- Yao Y., Tse J. S., Sun J., Klug D. D., Martonak R., and Iitaka T.: “Comment on “New Metallic Carbon Crystal””, *Phys. Rev. Lett.* **102**, No. 22, p. 229601 (2009). *
- Watanabe G., Sonoda H., Maruyama T., Katsuhiko S., Yasuoka K., and Ebisuzaki T.: “Formation of nuclear “pasta” in supernovae”, *Phys. Rev. Lett.* **103**, No. 12, pp. 121101-1–121101-4 (2009). *

口 頭 発 表 **Oral Presentations**

(国際会議等)

- Nomura S. and Iitaka T.: “Order-N electronic structure calculation of a Si quantum dot”, *International Symposium on Nanoscale Transport and Technology (IS-NTT2009)*, (NTT), Atsugi, Jan. (2009).
- Iitaka T.: “Large-scale quantum molecular dynamics simulation of 3-dimensional C60 polymers”, *3rd General Meeting of ACCMS-VO: Asian Consortium on Computational Materials Science - Virtual Organization*, (Center for Computational Materials Science, IMR, Tohoku University), Sendai, Feb. (2009).
- Tomono H., Iitaka T., and Tsumuraya K.: “GPU based Acceleration of First Principles Calculations”, *2009 APS March Meeting (MAR09)*, Pittsburgh, USA, Mar. (2009).
- Ohmori H., Maekawa K., Hachisu Y., Katahira K., Takizawa Y., Takahashi Y., Mizutani M., Kameyama Y., Sasaki M., Kato T., Kasuga H., and Sasaki C.: “Ultra-precision Micro-machining of Extreme Optics for Super-precision Observatory”, *MIRAI Short Seminar of Future of Micro-Precision Machining and Discussion on the 3rd MIRAI Joint Symposium on Micro-fabrication*, (UCB, Pan-pacific MIRAI), Davis, USA, June (2009).
- Iitaka T.: “GPU-accelerated Quantum Molecular Dynamics Simulation of 3-dimensional C60 Polymers”, *International Conference on Materials for Advanced Technologies 2009 (ICMAT 2009)*, (The Materials Research Society of Singapore), Singapore, Singapore, June–July (2009).
- Aoki M., Tomono H., Iitaka T., and Tsumuraya K.: “Ac-

celeration of orbital-free first principles calculation with GPU”, *International Conference on High Pressure Science and Technology, Joint AIRAPT-22 & HPCJ-50*, Tokyo, July (2009).

- Yagi T., Nagai T., Inoue T., Katayama Y., and Iitaka T.: “Earth science based on high-pressure and high-temperature neutron experiments: A new project using J-PARC”, *International Conference on High Pressure Science and Technology, Joint AIRAPT-22 & HPCJ-50*, Tokyo, July (2009).
- Tomono H., Aoki M., Iitaka T., and Tsumuraya K.: “GPU based acceleration of first principles calculation”, *International Conference on High Pressure Science and Technology, Joint AIRAPT-22 & HPCJ-50*, Tokyo, July (2009).
- Iitaka T.: “GPU-accelerated large-scale quantum molecular dynamics simulation of 3-dimensional C60 polymers”, *International Conference on High Pressure Science and Technology, Joint AIRAPT-22 & HPCJ-50*, Tokyo, July (2009).
- Hoshi T., Iitaka T., and Fyta M.: “Large scale simulation of quantum mechanical molecular dynamics for nanopolycrystalline diamond”, *International Conference on High Pressure Science and Technology, Joint AIRAPT-22 & HPCJ-50*, Tokyo, July (2009).
- Gao G., Oganov A. R., Ma Y., Bergara A., and Iitaka T.: “Novel high pressure phases of SnH₄”, *International Conference on High Pressure Science and Technology, Joint AIRAPT-22 & HPCJ-50*, Tokyo, July (2009).
- Tse J. S., Iitaka T., Kim E., and Yao Y.: “Structural search with evolution algorithm: The structure of solid H₂S at high pressure”, *International Conference on High Pressure Science and Technology, Joint AIRAPT-22 & HPCJ-50*, Tokyo, July (2009).
- Watson M. A.: “A mixed-precision matrix multiplication library for GPUs and its application to Quantum Chemistry calculations”, *Harvard-Riken Joint Symposium: Application of GPU Computation to Brain Science, Quantum Science, Astronomy, Fluid Dynamics and other sciences (HaRiken 09)*, Wako, Aug. (2009).
- Aoki M., Tomono H., Iitaka T., and Tsumuraya K.: “Accelerating Orbital-Free First Principles Calculation with Graphics Processing Unit”, *Harvard-Riken Joint Symposium: Application of GPU Computation to Brain Science, Quantum Science, Astronomy, Fluid Dynamics and other sciences (HaRiken 09)*, Wako, Aug. (2009).
- Aspuru-Guzik A.: “General-Purpose GPU computing for Quantum Chemistry”, *Harvard-Riken Joint Symposium: Application of GPU Computation to Brain Science, Quantum Science, Astronomy, Fluid Dynamics and other sciences (HaRiken 09)*, Wako, Aug. (2009).
- Hongo K.: “GPU acceleration of ab-initio quantum Monte Carlo simulations and its application to molecular crystals”, *Harvard-Riken Joint Symposium: Application of GPU Computation to Brain Science, Quantum Sci-*

- ence, Astronomy, Fluid Dynamics and other sciences (HaRiken 09), Wako, Aug. (2009).
- Tomono H., Aoki M., Iitaka T., and Tsumuraya K.: “GPU Based Acceleration of First Principles Calculation”, Harvard-Riken Joint Symposium: Application of GPU Computation to Brain Science, Quantum Science, Astronomy, Fluid Dynamics and other sciences (HaRiken 09), Wako, Aug. (2009).
- Stopa M. P.: “GPU for designing Semiconductor devices”, Harvard-Riken Joint Symposium: Application of GPU Computation to Brain Science, Quantum Science, Astronomy, Fluid Dynamics and other sciences (HaRiken 09), Wako, Aug. (2009).
- Iitaka T.: “GPU-accelerated Computing for Earth and Planetary High Pressure Science”, Harvard-Riken Joint Symposium: Application of GPU Computation to Brain Science, Quantum Science, Astronomy, Fluid Dynamics and other sciences (HaRiken 09), Wako, Aug. (2009).
- Tanaka H., Hattori T., Iitaka T., and Takata M.: “MEM charge density analysis by using GPU”, Harvard-Riken Joint Symposium: Application of GPU Computation to Brain Science, Quantum Science, Astronomy, Fluid Dynamics and other sciences (HaRiken 09), Wako, Aug. (2009).
- Nakasato N.: “Particle simulations with GPU”, Harvard-Riken Joint Symposium: Application of GPU Computation to Brain Science, Quantum Science, Astronomy, Fluid Dynamics and other sciences (HaRiken 09), Wako, Aug. (2009).
- Iitaka T.: “GPU-accelerated Massive Parallel Quantum Molecular Dynamics Simulation”, 5th Conference of Asian Consortium on Computational Materials Science (ACCMS-5), Hanoi, Viet Nam, Sept. (2009).
- Ohmori H., Uehara Y., Naruse T., Maekawa k., Hachisu Y., Katahira K., Mizutani M., Kasuga H., Kameyama Y., Sasaki M., Kato T., Wada S., Lin W., Umezu S., Komotori J., Ito N., Takizawa Y., Young R., Takahashi Y., Koizumi J., Andou T., Inada A., and Min S.: “Current Status of R and D Activities on Microfabrication in RIKEN Group for Critical Component Development”, 3rd MIRAI Forum (on Micro-Fabrication and Green Technology), Incheon, Korea, Oct. (2009).
- Otsuka T., Miyazaki T., Ohno T., Bowler D. R., and Gillan M. J.: “Theoretical study on total energy and atomic forces of hydrated DNA systems by CONQUEST code”, International Symposium of Electronic Structure Calculations: Theory, Correlated and Large Scale Systems and Numerical Methods, (The University of Tokyo), Tokyo, Dec. (2009).
- Zhang J., Kuo J., and Iitaka T.: “Hydrogen hydrate under high pressure”, 4th General Meeting of ACCMS-VO Asian Consortium on Computational Materials Science-Virtual Organization, (Center for Computational Materials Science, IMR, Tohoku University), Sendai, Jan. (2010).
- Hirano Y., Okimoto N., Yasuoka K., Suematsu M., and Yasui M.: “Molecular mechanisms how mercury inhibits water permeation of aquaporin-1: understanding by Molecular Dynamics Simulation”, Biophysical Society 54th Annual Meeting, San Francisco, USA, Feb. (2010).
- (国内会議)
- 飯高敏晃: “C60 ポリマーの分子動力学”, 第 11 回「プラズマと物質科学」研究討論会, (核融合研究所), 土岐, 1 月 (2009).
- 飯高敏晃: “Large-scale quantum molecular dynamics simulation of 3-dimensional C60 polymers”, 文部科学省科学研究費補助金特定領域研究「配列ナノ空間を利用した新物質科学: ユビキタス元素戦略」第 3 回領域会議, 東京, 1 月 (2009).
- 飯高敏晃: “3 次元 C60 ポリマーの有限温度ダイナミクス”, 日本物理学会第 64 回年次大会, 東京, 3 月 (2009).
- 伴野秀和, 青木優, 飯高敏晃, 圓谷和雄: “GPU による第一原理計算の高速化”, 日本物理学会第 64 回年次大会, 東京, 3 月 (2009).
- 星健夫, 飯高敏晃, Fyta M.: “ナノ多結晶ダイヤモンドの大規模電子構造計算”, 日本物理学会第 64 回年次大会, 東京, 3 月 (2009).
- 八木健彦, 永井隆哉, 井上徹, 片山芳則, 飯高敏晃: “J-PARC を用いた高温高压中性子実験と地球科学”, 日本地球惑星科学連合 2009 年大会, 千葉, 5 月 (2009).
- 飯高敏晃: “中性子実験と地球惑星科学に関連する物質の量子シミュレーション”, 日本地球惑星科学連合 2009 年大会, 千葉, 5 月 (2009).
- 伴野秀和, 青木優, 飯高敏晃, 圓谷和雄: “GPU による平面波基底第一原理計算の高速化”, 第 28 回日本シミュレーション学会大会, 東京, 6 月 (2009).
- 青木優, 伴野秀和, 飯高敏晃, 圓谷和雄: “第一原理計算の高速化”, 第 28 回日本シミュレーション学会大会, 東京, 6 月 (2009).
- 大塚教雄, 宮崎剛, 大野隆央, Bowler D. R., Gillan M. J.: “Large-scale DFT calculations of DNA systems with the linear-scaling DFT program CONQUEST”, 2nd Joint Workshop on Computational Science, 横浜, 7 月 (2009).
- 和田智之, 小川貴代, 前田康大, 戎崎俊一, 大森整: “JEM-EUSO プロジェクトにおけるライダー開発”, 第 27 回レーザーセンシングシンポジウム, (レーザー・レーダー研究会), 栃木県那須町, 9 月 (2009).
- 大塚教雄, 宮崎剛, 大野隆央, Bowler D. R., Gillan M. J.: “オーダー N 法を用いた DNA 系に対する大規模 DFT 計算: 全エネルギーと力と検証”, 第 3 回分子科学討論会, 名古屋, 9 月 (2009).
- 和田智之, 小川貴代, 戎崎俊一: “JEM-EUSO におけるライダーシステム”, 第 53 回宇宙科学技術連合講演会, (日本航空宇宙学会), 京都, 9 月 (2009).
- 飯高敏晃: “大規模量子分子動力学の GPU による加速”, 第一原理勉強会, (東京大学大学院理学系研究科常行研究室), 東京, 10 月 (2009).
- 飯高敏晃: “GPU-Accelerated Massively Parallel Quantum Molecular Dynamics Simulation”, 核融合科学研究所連携研

究推進センター客員セミナー, 土岐, 11月(2009).

飯高敏晃: “量子分子動力学の並列 GPU 計算による高速化”,
日本応用数理学会「行列・固有値問題の解法とその応用」
研究部会, 東京, 11月(2009).

飯高敏晃: “量子分子動力学の並列 GPU 計算による高速化”,
量子物理学・ナノサイエンス第 22 回セミナー, (東京工業
大学グローバル COE「ナノサイエンスを拓く量子物理学
拠点」), 東京, 11月(2009).

飯高敏晃: “GPGPU は「次世代スパコン」の敵か味方か”,
物性研究所 短期研究会 計算物理学, (東京大学物性研究所),
柏, 12月(2009).

平野秀典, 沖本憲明, 泰岡顕治, 末松誠, 泰地真弘人, 安井正人:
“水銀によるアクアポリンの水透過阻害機構の解明”, 日本
薬学会第 130 年会, (日本薬学会), 岡山, 3月(2010).