

Poster Presentations

1. “Understanding the tribological behavior of friction modifiers in DLC/DLC systems using a Tight-Binding Quantum Chemical Method”

E. Deguillard¹, S. Loehlé¹, M. Kubo²

¹ *TOTAL, TOTAL Marketing & Services, Centre de Recherche de Solaize, BP22 69360 Solaize - France*

² *Fracture and Reliability Research Institute, Graduate School of Engineering, Tohoku University, 6-6-11, Aoba, Aramaki, Aoba-ku, Sendai 980-8579, Japan*

2. “Pressure-induced amorphization of crystalline polymer studies by coarse-grain model”

Takanori Kai and Yasuhiro Senda

Department of Applied Science, Yamaguchi University, Yamaguchi, 755-8611, Japan

3. “Demon-based Monte Carlo sampling to accelerate the simulations of classical spin systems”

Kazuhito Shida

New Industry Creation Hatchery Center, Tohoku University, Sendai, Japan

4. “Implementation of spin-orbit coupling in TOMBO code”

Takeru Nakashima and Kaoru Ohno

Department of Physics, Yokohama National University, Yokohama 240-8501, Japan

5. “Implementation of force calculation in Hartree-Fock approximation in TOMBO code”

Shuichi Uehara and Kaoru Ohno

Department of Physics, Yokohama National University, Yokohama 240-8501, Japan

6. “Extension of hyperfine calculation to crystal systems in TOMBO Ver.2”

Hiroyuki Terada and Kaoru Ohno

*Department of Physics, Yokohama National University, Yokohama
240-8501, Japan*

7. “Calculation of the photo absorption spectra using the GW approximation for the (N-1)-electron system”

Tomoharu Iso and Kaoru Ohno

*Department of Physics, Yokohama National University, Yokohama
240-8501, Japan*

8. “First-principles calculations of core electron binding energies for insulators and semiconductors with the one-shot GW method”

Tsubasa Aoki and Kaoru Ohno

*Department of Physics, Yokohama National University, Yokohama
240-8501, Japan*

9. “A first-principles based approach for phase field crystal model using a total energy expression involving the atomic electron charge density”

Swastibrata Bhattacharyya¹, Kaoru Ohno¹, and Ryoji Sahara²

¹ *Department of Physics, Yokohama National University, 79-5 Tokiwadai,
Hodogaya, Yokohama 240-8501, Japan*

² *National Institute for Materials Science (NIMS), 1-2-1 Sengen, Tsukuba
305-0047, Japan*

10. “Validity of the quasi-equilibrium approach to nonequilibrium phonon dynamics”

Shota Ono

*Department of Electrical, Electronic, and Computer Engineering, Gifu
University, Gifu 501-1193, Japan*

11. “Comprehensive Studies on the Tri-iodide Reduction Activity of Shape- and Composition- Controlled PtFe Nanostructures: Their Combination as the Counter Electrode in Dye-Sensitized Solar Cells”

Hung-Lung Chou,¹ Pei-Jen Chang,² Kum-Yi Cheng,² Shang-Wei Chou,²
Jing-Jong Shyue,² Ya-Yun Yang,⁴ Hui-Lung Chen,⁵ Pi-Tai Chou^{2,3}

¹ *Graduate Institute of Applied Science & Technology, National Taiwan*

University of Science and Technology, Taipei, Taiwan, 10617;

² Department of Chemistry, National Taiwan University, Taipei, Taiwan, 10617;

³ Center of Emerging Material and Advanced Devices, National Taiwan University, Taipei, Taiwan, 10617;

⁴ Instrumentation Center, National Taiwan University, Taipei, Taiwan;

⁵ Department of Chemistry and Institute of Applied Chemistry, Chinese Culture University, Taipei, Taiwan, 111;

12. “Energy conversion efficiency of organic photovoltaic cells: heterojunction of peanut-shaped fullerene polymer and zinc phthalocyanine”

Kousei Tanikawa¹, Yusuke Noda², Shota Ono³, and Kaoru Ohno¹

¹ Department of Physics, Yokohama National University, Yokohama 240-8501, Japan

² Materials Research by Information Integration Initiative (M²I), National Institute for Materials Science, 1-2-1 Sengen, Tsukuba 305-0047, Japan

³ Department of Electrical, Electronic, and Computer Engineering, Gifu University, Gifu 501-1193, Japan

13. “First-principles electronic structure calculation of Zintl compound Na₂ZnSn₅”

J. Hirata, K. Akai, K. Kishimoto, H. Kurisu, T. Koyanagi, S. Yamamoto
Graduate School of Sciences and Technology for Innovation, Yamaguchi University, 2-16-1 Tokiwadai, Ube-shi, Yamaguchi-ken 755-8611

14. “Band spin splitting of LaMnO₃ with lower symmetries”

Takuya Okugawa¹, Yusuke Noda², Kaoru Ohno², and Shinichiro Nakamura³

¹ Department of Physics, Yokohama National University, 79-5 Tokiwadai, Hodogaya, Yokohama 240-8501, Japan

² Department of Life Science and Applied Chemistry, Nagoya Institute of Technology, Gokiso-cho, Showa-ku, Nagoya, Aichi, 466-8555, Japan

³ RIKEN Innovation Center, Nakamura Laboratory, 2-1 Hirosawa, Wako, Saitama 351-0198, Japan

15. “Clustering, magnetic feature and atomic migration in the Fe₈₅Si₂B₉P₄ amorphous alloy”

Yaocen Wang^{1*}, Akira Takeuchi¹, Akihiro Makino¹, Yoshiyuki Kawazoe²

¹ *Institute for Materials Research, Tohoku University, 980-8577, Sendai, Japan*

² *New Industry Creation Hatchery Center, Tohoku University, 980-8579, Sendai, Japan*

16. “Stability of analysis of NdFe₁₂-based compounds as promising new high performance permanent magnet materials - Effect of Zr”

Arkapol Saengdeejing¹ and Ying Chen¹

¹ *Fracture and Reliability Research Institute, Graduate School of Engineering, Tohoku University*

17. “A Comparison of Thermoelectric Properties for Simulation Results and Experiment Data of Bulk Silicon”

Ken-Ming Lin and Y. H. Tang

Department of Physics, National Central University, Taiwan

18. “Effect of substrates on the phonon transport in graphene”

Arun S Nissimagoudar¹, Rinkle Juneja¹, Hisayoshi Ooshima³, Norikazu Hosokawa³, Yoshiyuki Kawazoe², and Abhishek K. Singh¹

¹ *Indian Institute of Science, Bangalore, India*

² *New Industry Creation Hatchery Center, Tohoku University, Japan*

³ *Fundamental Laboratory, Denso, Japan*

19. “Use of Bond-order Empirical Potentials in the Study of Lowest Energy Structures of Carbon Clusters”

Icuk Setiyawati, T.W. Yen, Y. H. Tang and S. K. Lai

Department of Physics, National Central University, Zhong-Li, Taiwan

20. “Adsorption Property of Water Molecule on Belite Surface”

Ryoji Sakurada¹, Masami Uzawa², Yoshifumi Hosokawa³, Syun-ichiro Uchida³, Yoshiyuki Kawazoe⁴, Aaditya Manjanath⁵, and Abhishek

Kumar Singh⁵

¹ *Dept. of Civil Engineering, National Institute of Technology, Akita College, JAPAN*

² *College of Industrial Technology, Nihon University, JAPAN*

³ *Central Research Laboratory, Taiheiyo Cement Co., Ltd., JAPAN*

⁴ *New Industry Creation Hatchery Center, Tohoku University, JAPAN*

⁵ *Materials Research Centre, Indian Institute of Science, INDIA*

21. "Role of impurity in oxidation resistance of Ti : *Ab initio* DFT study"

Somesh Kr. Bhattacharya, Ryoji Sahara, Tomonori Kitashima, Ayako Ikeda, Kyosuke Ueda, and Takayuki Narushima

Computational Structural Materials Design group, Research Center for Structural Materials, National Institute for Materials Science (NIMS), Tsukuba, Ibaraki, Japan

22. "Chemical forms of Molybdenum ion in nitric acid solution studied using XAFS spectroscopy and first-principles calculations"

T. Sato¹, Y. Sawada¹, S. Watanabe¹, M. Nakaya¹, M. Yoshino¹, T. Nagasaki¹, T. Yoshida², J. Onoe¹

¹ *Department of Materials, Physics and Energy Engineering, Nagoya University, Japan*

² *The OCU Advanced Research Institute for Natural Science and Technology, Osaka City University, Japan*

23. "Ionic Conductivity in Thin-Film Ionic Liquid: A Molecular Dynamics Study"

Ida Bagus Hendra P.¹, Yusuke Ootani¹, Takeshi Nishimatsu¹, Yuji Higuchi¹, Nobuki Ozawa¹, Shingo Maruyama², Yuji Matsumoto², and Momoji Kubo¹

¹ *Institute for Materials Research, Tohoku University, 2-1-1 Katahira, Aoba-ku, Sendai 980-8577, Japan*

² *Department of Applied Chemistry, Tohoku University, 6-6-07 Aramaki Aza Aoba, Aoba-ku, Sendai 980-8579, Japan*

24. "Theoretical insights into the Design of 2D-material based van der Waals heterostructures - A first principles study"

K. Iyakutti*^{1,2}, R. Lavanya², E. Mathan Kumar³, V. J. Surya¹, R. Thapa³ and Y. Kawazoe⁴

¹*Department of Physics and Nanotechnology, SRM University, Kattankulathur, Tamilnadu-603203, India.*

²*Department of Renewable Energy Science, M.S University, Thirunelveli, Tamilnadu-627012, India.*

³*SRM Research Institute, SRM University, Kattankulathur, Tamil Nadu 603203, India*

⁴*New Industry Creation Hatchery Center, Tohoku University, Aramaki, Sendai 980-8579, Japan.*

25. “Roles of Zeolite Confinement and Cu–O–Cu Angle on the Direct Conversion of Methane to Methanol by [Cu₂O]²⁺-exchanged AEI, CHA, AFX, and MFI Zeolites”, Muhammad Haris Mahyuddin,¹ Aleksandar Staykov,² Yoshihito Shiota,¹ and Kazunari Yoshizawa¹

¹ *Institute for Materials Chemistry and Engineering, Kyushu University, Fukuoka 819-0395, Japan*

² *International Institute for Carbon-Neutral Energy Research, Kyushu University, Fukuoka 819-0395, Japan*