

Poster Presentations

1. "Investigation of induced bond distortion in graphene leading to quasi 2D-structured materials like penta graphene"

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2. "GW without BSE method: simple and accurate calculation of photoabsorption spectra for spin polarized systems"

Tomoharu Isobe¹, Riichi Kuwahara², and Kaoru Ohno¹

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"Searching of suitable cationic dopants for solar absorber material CZTS/Se using first-principles method"

3. "Origin of the breaking of general term ordering for diatomic boron and carbon molecules"

Daisuke Yoshida and Hannes Raebiger

Department of Physics, Yokohama National University

4. "Thermodynamic assessment of the carbon-zirconium system"

Theresa Davey^{1,2}, Thomas A. Mellan¹, Suzana G. Fries³, Michael W. Finnis^{1,4}

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5. “Carbon Allotropes as anode material for Li-ion battery”
A. Rajkamal^a, E. Mathan Kumar^a, Akhil T. Shettigar^a, Noejung Park^b and Ranjit Thapa^a
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6. “Searching of suitable cationic dopants for solar absorber material CZTS/Se using first-principles method”
M. V. Jyothirmai and Ranjit Thapa
SRM Research Institute & Department of Physics and Nanotechnology, SRM University, Kattankulathur 603203, Tamil Nadu, India

7. “Homonuclear boron bond in carbon allotropes identify as a universal gas sensor: Conversion of gas molecules”
Vanshree Parey^{1,2}, N. K. Gaur², Ranjit Thapa¹
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8. “Doping enhanced ferromagnetism and induced half-metallicity in CrI₃ monolayer”
Hongbo Wang^{1,2}, Fengren Fan¹, Shasha Zhu¹, and Hua Wu^{1*}
¹ *Laboratory for Computational Physical Sciences, State Key Laboratory of Surface Physics, and Department of Physics, Fudan University, Shanghai, China*
² *Department of Physics, University of Jinan, Jinan, Shandong, China*

9. “Cooperatively enhanced catalytic properties of Ti@Al(100) near-surface alloy for aluminum hydrogenation ”
M. M. Zheng^{1,2}, G. Chen²

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10. “Investigation of $\text{AlCl}_4\text{-AlCl}_3$ clusters intercalated in graphite layer for rechargeable Al-ion battery”

Hung-Lung Chou

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11. “First-principles Understanding of Ferromagnetic Mechanism in Ge-based DMSs”

H. Shinya^{1,3}, T. Fukushima², A. Masago³, K. Sato⁴, H. Katayama-Yoshida⁵, and K. Ohno¹

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12. “Vibration Infrared Spectra for Large Molecules: Development and Application of FMO-PCM Method”

Hiroya Nakata¹, Dmitri G. Fedorov².

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13. “Molecular Dynamics Simulation on Plastic Deformation Mechanism of Iron Material in Supercritical Aqueous Environment”

Qian Chen, Jingxiang Xu, Yusuke Ootani, Nobuki Ozawa, and Momoji Kubo

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Aoba-ku, Sendai 980-8577, Japan)

14. “Coarse-Grained Molecular Dynamics Simulation on the Wear Mechanism of Cyclic Polymer Brush”

Zhongmin Liu, Shuichi Uehara, Jingxiang Xu, Yusuke Ootani, Nobuki Ozawa, and Momoji Kubo

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15. “Investigation on Wear Mechanism of DLC Coating under Water Lubrication by Molecular Dynamics Simulation”

Jing Zhang¹, Yang Wang¹, Jingxiang Xu¹, Yusuke Ootani¹, Nobuki Ozawa¹, Koshi Adachi², and Momoji Kubo¹

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16. “Simulation of powder bed preparation in additive manufacturing”

Keiko Kikuchi, Naoyuki Nomura, Akira, Kawasaki

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17. “Optical investigations of Pr/Ce-doped APLF glasses for scintillator applications”

J. F. Gabayno^{1,3}, Y. Minami¹, M. J. F. Empizo¹, K. Yamanoi¹, M. V. Luong¹, T. Shimizu¹, N. Sarukura¹, and T. Murata²

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18. “UV-Vis/XAFS spectroscopic and first-principles studies of the chemical forms of ruthenium and palladium ions in nitric acid solution”

T. Sato¹, S. Watanabe¹, M. Nakaya¹, M. Yoshino¹, T. Nagasaki¹, T.

Yoshida², and J. Onoe¹

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19. “Stability of Supported Single-Atom Catalysts: Insight from Density Functional Theory”

Nguyen-Dung Tran¹ and Stefano Fabris^{2, 3}

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20. “First-principles and spectroscopic studies on the sorption properties of Prussian blue for Ru, Rh, Pd and Mo ions in nitric acid solution”

S. Watanabe¹, Y. Sawada², T. Sato², M. Nakaya¹, M. Yoshino¹, T. Nagasaki¹, R. Mishima³, M. Harigai³, Y. Inaba³, K. Takeshita³, J. Onoe¹

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21. “Accurate ab-initio calculations of hyperfine structures of some atoms and radicals”

Hiroyuki Terada and Kaoru Ohno

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22. “Growth of microstructures in NiAl alloy from first principles based phase field method”

Swastibrata Bhattacharyya¹, Ryoji Sahara², Kaoru Ohno¹

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23. “Theoretical Study on Structure Change from sp^3 to sp^2 Carbon on Diamond-like Carbon Surface by the Oxidation Reaction”

Shandan Bai¹, Jingxiang Xu², Nobuki Ozawa², Momoji Kubo²

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24. “Electronic structure study on Zintl compound Na_2ZnSn_5 by using Wannier functions”

J. Hirata, K. Akai, K. Kishimoto, H. Kurisu, T. Koyanagi, S. Yamamoto
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25. “A neutron scintillator based on praseodymium-doped complex fluoro-oxide glass”

M. J. F. Empizo¹, M. Cadatal-Raduban², T. Murata³, Y. You¹, Y. Minami¹, K. Kawano¹,
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26. “Optical damage assessment of gamma-ray irradiated bulk crystals and glasses”

Y. Lai¹, J. L. F. Gabayno^{1,2}, K. Yamanoi¹, M. J. F. Empizo¹, Y. Minami¹, B. G.

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27. “Design of a n-ZnO/p-Si heterojunction device for photodetector applications”

R. C. Veloz¹, M. C. A. Angub¹, H. A. F. Husay², E. J. C. D. Solibet², M. J. F. Empizo³, K. Kawano³, N. Sarukura¹, A. A. Salvador^{1,2}, E. S. Estacio^{1,2}, and A. S. Somintac^{1,2}

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28. “Structure and application of Lithium-Cation Endohedral C₆₀ Fullerene”

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29. “Structural and optical properties of ZnO-PVP composites for potential phosphor-based applications”

Verdad C. Agulto¹, Melvin John F. Empizo¹, Keisuke Kawano¹, Yuki Minami¹, Kohei Yamanoi¹, Nobuhiko Sarukura¹, Allan Christopher Yago², and Roland V. Sarmago³

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30. “First-Principles Study of Belite Activation by Doping of a Trace Element”
Ryoji Sakurada¹, Masami Uzawa², Yoshifumi Hosokawa³, Syun-ichiro Uchida³, Yoshiyuki Kawazoe⁴, Aaditya Manjanath⁵, and Abhishek Kumar Singh⁵

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31. “Synthesis of Zinc Oxide Nanoparticles for Functionalization of Fabrics: (Superhydrophobic & UV-Protection)”

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32. “Theoretical prediction of two-dimensional functionalized MXene nitrides as topological insulators”

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