

センター利用による研究成果

—平成30年度計算機利用結果報告書から—

【1501 生活科学一般】

1. A. K. Sharma, W. M. C. Sameera, Y. Takeda, S. Minakata : A computational study on the mechanism and origin of the regioselectivity and stereospecificity in Pd/SIPr-catalyzed ring-opening cross-coupling of 2-arylaziridines with aryl-boronic acids : ACS Catal., 2019

【2103 マイクロ・ナノデバイス】

2. 山口 謙祐、ムルガナタン マノハラン、水田 博、田部 道晴、モラル ダニエル：第一原理計算を用いた外部電場による Si ナノ構造上の不純物への影響：第 66 回応用物理学会春季学術講演会要旨, 2019

【4104 基礎解析学】

3. Kengo NAKAI, Yoshitaka SAIKI : Machine-learning inference of fluid variables from data using reservoir computing : Phys. Rev. E, Vol.98, No.2, pp.023111 - 023116, 2018

【4305 原子・分子・量子エレクトロニクス・プラズマ】

4. Jun Tokimoto, Shunji Tsuchiya, and Tetsuro Nikuni : Excitation of Higgs Mode in Superfluid Fermi Gas in BCS-BEC Crossover : Journal of Physical Society of Japan, Vol.88, No.023601, 2019

【4306 生物物理・化学物理】

5. Ryuma Sato, Hirotaka Kitoh-Nishioka, Koji Ando, Takahisa Yamato : Electron Transfer Pathways of Cyclobutane Pyrimidine Dimer Photolyase Revisited : The Journal of Physical Chemistry B, Vol.122, No.27, pp.6912 - 6921, 2018

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【4601 物理化学】

8. Sandeep K. Reddy, Raphael Thiriaux, Bethany A. Wellen Rudd, Lu Lin, Tehseen Adel, Tatsuya Joutsuka, Franz M. Geiger, Heather C. Allen, Akihiro Morita, and Francesco Paesani : Bulk Contributions Modulate the Sum-Frequency Generation Spectra of Interfacial Water on Model Sea-Spray Aerosols : Chem, Vol.4, No.7, pp.1629 - 1644, 2018
9. Tatsuya Joutsuka and Akihiro Morita : Electrolyte and Temperature Effects on Third-Order Susceptibility in Sum Frequency Generation Spectroscopy of Aqueous Salt Solutions : J. Phys. Chem. C, Vol.122, No.21, pp.11407 - 11413, 2018

【4801 機能材料・デバイス】

10. Miho Itoi, Atsushi Okazawa, Jun-ichi Yamaura, Sachiko Maki, Tokutaro Komatsu, Isabelle Maurin, Epiphane Codjovi, Kamel Boukhedadden, and Norimichi Kojima : Structural Insight into Order-Disorder Transition and Charge-Transfer Phase Transition in an Iron Mixed-Valence Complex ($n\text{-C}_3\text{H}_7\text{)}_4\text{N}[\text{Fe}^{\text{II}}\text{Fe}^{\text{III}}(\text{d}\text{t}\text{o})_3]$ with a Two-Dimensional Honeycomb Network : Inorganic

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【4902 薄膜・表面界面物性】

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【4905 工学基礎】

12. Shugo Yasuda : Synchronized molecular-dynamics simulation of the thermal lubrication of an entangled polymeric liquid : Polymers, Vol.11, pp.131-, 2019
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【5001 機械材料・材料力学】

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【5004 流体工学】

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【5501 化工物性・移動操作・単位操作】

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