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発表者	掲載誌	題名
Y. Saito, K. Asaka	Recent Developments in Atomic Force Microscopy and Raman Spectroscopy for Materials Characterization (2021, IntechOpen)	Raman Features of Linear-Carbon-Chain and Multiwall Carbon Nanotube Composites
Yahachi Saito	<i>J. Vac. Sci. Technol. B</i> , 40 (2022) 012803 (6p)	Field ion microscopy images of multilayered graphene and graphene oxide
K. Asaka, K. Yamauchi, Y. Saito	<i>Diamond & Relat. Mater.</i> , 124 (2022) 108907 (5p)	Critical current density for layer-by-layer breakdown of a multiwall carbon nanotube
S. Tanaka, T. Yoshida, K. Watanabe, Y. Matsumoto, T. Yasuike, D. Novko, M. Petrović, M. Kralj	<i>ACS Photonics</i> , 9 (2022) <i>in press</i> , https://doi.org/10.1021/acsp Photonics.1c01454	Ultrafast Plasmonic Response Ensured by Atomic Scale Confinement
M. Raczkowski, F. F. Assaad, M. Imada	<i>Phys. Rev. B</i> , 103 (2021) 125137	Local moments versus itinerant antiferromagnetism: Magnetic phase diagram and spectral properties of the anisotropic square lattice Hubbard model
Y. Nomura, M. Imada	<i>Phys. Rev. X</i> , 11 (2021) 031034	Dirac-type nodal spin liquid revealed by refined quantum many-body solver using neural-network wave function, correlation ratio, and level spectroscopy
Masatoshi Imada	<i>J. Phys. Soc. Jpn.</i> , 90 (2021) 074702	Resonant Inelastic X-Ray Scattering Spectra of Cuprate Superconductors Predicted by Model of Fractionalized Fermions
Masatoshi Imada	<i>J. Phys. Soc. Jpn.</i> , 90 (2021) 111009	Charge Order and Superconductivity as Competing Brothers in Cuprate High- T_c Superconductors
M. Charlebois, J.-B. Morée, K. Nakamura, Y. Nomura, T. Tadano, Y. Yoshimoto, Y. Yamaji, T. Hasegawa, K. Matsuhira, M. Imada	<i>Phys. Rev. B</i> , 104 (2021) 075153	<i>Ab initio</i> derivation of low-energy Hamiltonians for systems with strong spin-orbit interaction: Application to $\text{Ca}_5\text{Ir}_3\text{O}_{12}$
F. Imoto, M. Imada, A. Oshiyama	<i>Phys. Rev. Research</i> , 3 (2021) 033198	Order-N orbital-free density-functional calculations with machine learning of functional derivatives for semiconductors and metals
Y. Yamaji, T. Yoshida, A. Fujimori, M. Imada	<i>Phys. Rev. Research</i> , 3 (2021) 043099	Hidden self-energies as origin of cuprate superconductivity revealed by machine learning
X. Zhou, W.-S. Lee, M. Imada, N. Trivedi, P. Phillips, H.-Y. Kee, P. Torma, M. Eremets	<i>Nat. Rev. Phys.</i> , 3 (2021) 462	High-temperature superconductivity
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大門 寛, 桃野浩樹, 松田博之, L. Tóth, 益田 有, 森口幸一, 小粥啓子, 竹内走一郎, 橋本由介, 松下智裕	表面と真空 「マイクロビームアナリシス 技術部会特集号」, 64 (2021) 452-457 DOI: https://doi.org/10.1380/vss.64.452	原子分解能ホログラフィー顕微鏡の開発
S. Takeuchi, Y. Hashimoto, H. Daimon, T. Matsushita	<i>Journal of Electron Spectroscopy and Related Phenomena</i> , <i>in print</i>	High-precision atomic image reconstruction from photoelectron hologram of O on W(110) by SPEA-L1

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Keiko Nishikawa	<i>Bull. Chem. Soc. Jpn.</i> , 94 (2021) 2170-2186	The Solution Chemistry of Mixing States Probed via Fluctuations: a Direct Description of Inhomogeneity in Mixing
N. Yoshida, M. Matsugami, Y. Harano, K. Nishikawa, F. Hirata	<i>J.</i> , 4 (2021) 698-726	Structure and Properties of Supercritical Water: Experimental and Theoretical Characterizations
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Y. Doi, A. Takano, Y. Matsushita	<i>Polymer J.</i> DOI 10.1038/s41428-021-00530-x	Preparation and Distorted cylindrical Morphology of Block Copolymers Consisting of Flexible and Semiflexible Blocks
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J. Suzuki, M. Suzuki, A. Takano, Y. Matsushita	<i>Macromol. Theory. Simul.</i> , 2021 https://doi.org/10.1002/mats.202100015	Cylindrical Super-Lattice Structures with Three-Contrasts from Pentablock Binary Blends Studied by Monte Carlo Simulation

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榎木勝徳, 高橋宏太, 三富崇永, 大谷博司	鉄と鋼	鉄鋼における熱力学物性値の電子論計算とFe-Mo-B三元系理論状態図への応用
A. Saengdeejing, Y. Chen, O. Takeda, M. Enoki, S. Sugimoto, H. Ohtani, A. Taichi	Calphad	Sm-Ti binary thermodynamic database and phase diagram
H. Tanaka, T. Yagasaki, M. Matsumoto	<i>J. Chem. Phys.</i> , 155 (2021) 214502 (12 pages)	On the role of intermolecular vibrational motions for ice polymorphs. III. Mode characteristics associated with negative thermal expansion
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Yukihiro Ozaki	<i>Anal. Sci.</i> https://doi.org/10.2116/analsci.20R008	Infrared Spectroscopy — Mid-infrared, Near-infrared, and Far-infrared/Terahertz Spectroscopy
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M. Ishigaki, A. Ito, R. Hara, S. Miyazaki, K. Murayama, K. Yoshikiyo, T. Yamamoto, Y. Ozaki	<i>Anal. Chem.</i> , 93 (2021) 2758-2766	Method of Monitoring the Number of Amide Bonds in Peptides Using Near-Infrared Spectroscopy
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P. Pienpinijtham, Y. Kitahama, Y. Ozaki	<i>J. Raman Spectrosc.</i> , DOI: 10.1002/jrs.618, Special issue-invited review	Electric field analysis, polarization, excitation wavelength dependence, and novel applications of tip-enhanced Raman scattering

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Y. Morisawa, Y. Higaki, Y. Ozaki	Published as part of The Journal of Physical Chemistry virtual special issue, "125 Years of The Journal of Physical Chemistry": <i>J. Phys. Chem., A</i> , 2021, doi.org/10.1021/acs.jpca.1c05688	Far-Ultraviolet Spectroscopy and Quantum Chemical Calculation Studies of the Conformational Dependence on the Electronic Structure and Transitions of Cyclohexane, Methyl and Dimethyl Cyclohexane, and Decalin; Effects of Axial Substitutions on the Electronic Transitions
Y. Ozaki, K. B. Beć, Y. Morisawa, S. Yamamoto, I. Tanabe, C. W. Huck, T. Hofer	<i>Chem. Soc. Rev.</i> , 2021, DOI: 10.1039/d0cs01602k	Recent advances in quantum chemical approach in molecular spectroscopy of the condensed phase
M. A. Czarnecki, Y. Morisawa, Y. Katsumoto, T. Takaya, S. Singh, H. Sato, Y. Ozaki	<i>Phys. Chem. Chem. Phys.</i> , 23 (2021) 19188	Solvent Effect on Competition Between Weak and Strong Interactions in Phenol Solutions Studied by Near-infrared Spectroscopy and DFT Calculations
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S. Singh, M. Majer, M. A. Czarnecki, Y. Morisawa, Y. Ozaki	<i>Applied Spectroscopy</i> , 2021, DOI: 10.1177/ 00037028211052302	Solvent Effect on Assembling and Interactions in Solutions of Phenol: Infrared Spectroscopic and Density Functional Theory Study
P. M. Witkowski, C. Brosseau, Y. Ozaki, A. Królikowska, eds.	<i>Front. Chem.</i> , doi.org/10.3389/fchem. 2021.784735	Novel SERS-Active Materials and Substrates: Sensing and (Bio) applications
L. Zhu, P. Li, H. Sun, X. Han, Y. Xu, X. Wang, B. Liu, Y. Ozaki, B. Zhao	<i>Nanoscale</i> , DOI: 10.1039/d1nr06250f	An investigation of the effect of high-pressure on charge transfer in dye-sensitized solar cells based on surface-enhanced Raman spectroscopy

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X.-X. Han, R. S. Rodriguez, C. L. Haynes, Y. Ozaki, B. Zhao	<i>Nature Rev. Methods Prim.</i> , 2022, doi.org/10.1038/s43586-021-00083-6	
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N. Ueno, M. Takegoshi, A. Zaitceva, Y. Ozaki, Y. Morisawa	<i>J. Chem. Phys.</i> , 156 (2022) 074705, Invited; Special issue; <i>JCP Special Topic on the Chemical Physics of the Electrode–Electrolyte Interface</i>	Experimental verification of increased electronic excitation energy of water in hydrate-melt water by attenuated total reflection-far-ultraviolet spectroscopy
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Yukihiro Ozaki	<i>NIR News</i> , 2022, DOI: 10.1177/ 09603360211067093	NIR spectroscopy — What a wonderful world!
E. Mitani, Y. Ozaki, H. Sato	<i>Polymer</i> , 246 (2022) 124725	Two types of C—O…HO hydrogen bonds and OH…OH (dimer, trimer, oligomer) hydrogen bonds in PVA with 88% saponification/PMMA and PVA with 99% saponification/PMMA blends and their thermal behavior studied by infrared spectroscopy
Y. Wang, C. Cheng, R. Ma, Z. Xu, Y. Ozaki	<i>Analyst</i> , DOI: 10.1039/d2an00035k	<i>In situ</i> SERS monitoring of intracellular H ₂ O ₂ in single living cells based on label-free bifunctional Fe ₃ O ₄ @Ag nanoparticles

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