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Temperature Distribution Design Based on Variable Lattice Density Optimization and Metal Additive Manufacturing	Ueno, Akira; Guo, Honghu; Takezawa, Akihiro; Moritoyo, Ryota; Kitamura, Mitsuru	SYMMETRY-BASEL	2021	JUL	13	7	
Development and Application of a ReaxFF Reactive Force Field for Cerium Oxide/Water Interfaces	Brugnoli, Luca; Menziani, Maria Cristina; Urata, Shingo; Pedone, Alfonso	JOURNAL OF PHYSICAL CHEMISTRY A	2021	JUL	125	25	5693-5708
In situ transmission infrared spectroscopy of plasma-assisted CO ₂ hydrogenation on ZnO: Role of catalyst support materials	SAITO Atsushi, SHENG Zunrong, KIM Dae-Yeong, IMAMURA Yutaka, NOZAKI Tomohiro	International Journal of Plasma Environmental Science and Technology (Web)	2021	JUL	15	2	Page. ROMBU NNO.e02008 (WEB ONLY)
Self-assembly of the cationic surfactant n-hexadecyl-trimethylammonium chloride in methyltrimethoxysilane aqueous solution: classical and reactive molecular dynamics simulations	Urata, Shingo; Kuo, An-Tsung; Murofushi, Hidenobu	PHYSICAL CHEMISTRY CHEMICAL PHYSICS	2021	JUL	23	26	14486-14495
Photo-on-Demand Base-Catalyzed Phosgenation Reactions with Chloroform: Synthesis of Arylcarbonate and Halocarbonate Esters	Hashimoto, Yuka; Hosokawa, Sasuga; Liang, Fengying; Suzuki, Yuto; Dai, Namin; Tana, Gegen; Eda, Kazuo; Kakiuchi, Toshifumi; Okazoe, Takashi; Harada, Hidefumi; Tsuda, Akihiko	JOURNAL OF ORGANIC CHEMISTRY	2021	JUL	86	14	9811-9819
Evaluation of the Effect of Art Content on Mental States Using Mirror Display with AR Function	NAKATSU Ryohei, TOSA Naoko, NIIYAMA Satoshi, SAKURAI Shigeki, KUSUMI Takashi	Proceedings of the International Display Workshops (Web)	2021	JUL	28		Page. ROMBU NNO.VHF 5-3 (WEB ONLY)
Recent Standardization Activities for Electronic Displays in IEC TC 110—Following Technology Development —	HYODO Kei, SHIBAHARA Yoshi, UEHARA Shin	Proceedings of the International Display Workshops (Web)	2021	JUL	28		Page. ROMBU NNO.DES 5-1 (WEB ONLY)
Structural origin of thermal shrinkage in soda-lime silicate glass below the glass transition temperature: A theoretical investigation by microsecond timescale molecular dynamics simulations	Shimizu, Masahiro; Murota, Teppei; Urata, Shingo; Takato, Yoichi; Hamada, Yuya; Koike, Akio; Shimotsuma, Yasuhiko; Fujita, Koji; Miura, Kiyotaka	JOURNAL OF CHEMICAL PHYSICS	2021	JUL	155	4	
Exploring the crystallization path of lithium disilicate through metadynamics simulations	Lodesani Federica, Tavanti Francesco, Tavanti Francesco, Menziani Maria Cristina, Maeda Kei, Takato Yoichi, Urata Shingo, Pedone Alfonso	Physical Review Materials	2021	JUL	5	7	75602
Mathematical model and numerical analysis method for dynamic fracture in a residual stress field	Hirobe Sayako, Imakita Kenji, Aizawa Haruo, Kato Yasumasa, Urata Shingo, Oguni Kenji	Physical Review. E	2021	AUG	104	2	25001

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Simulation of Catastrophic Failure in a Residual Stress Field	Hirobe, Sayako; Imakita, Kenji; Aizawa, Haruo; Kato, Yasumasa; Urata, Shingo; Oguni, Kenji	PHYSICAL REVIEW LETTERS	2021	AUG	127	6	
Mechanism of material removal through transient and selective laser absorption into excited electrons in fused silica	Yoshizaki, Reina; Ito, Yusuke; Yoshitake, Shunya; Wei, Chaoran; Shibata, Akihiro; Nagasawa, Ikuo; Nagato, Keisuke; Sugita, Naohiko	JOURNAL OF APPLIED PHYSICS	2021	AUG	130	5	
Void Engineering in Silica Glass for Ultralow Optical Scattering Loss	Ono, Madoka	JOURNAL OF LIGHTWAVE TECHNOLOGY	2021	AUG	39	16	5258-5262
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Tuning the mechanical toughness of the metal nanoparticle-implanted glass: The effect of nanoparticle growth conditions	Ono, Madoka; Miyasaka, Satoshi; Takato, Yoichi; Urata, Shingo; Hayashi, Yasuo	JOURNAL OF THE AMERICAN CERAMIC SOCIETY	2021	OCT	104	10	5341-5353
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Molecular dynamics study on the co-doping effect of Al ₂ O ₃ and fluorine to reduce Rayleigh scattering of silica glass	Urata, Shingo; Nakamura, Nobuhiro; Tada, Tomofumi; Hosono, Hideo	Journal of the American Ceramic Society	2021	OCT	104	10	5001-5015
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Methyl to trifluoromethyl substitution as a strategy to increase the membrane permeability of short peptides	Ono, Takahiro; Aikawa, Kohsuke; Okazoe, Takashi; Morimoto, Jumpei; Sando, Shinsuke	ORGANIC & BIOMOLECULAR CHEMISTRY	2021	NOV	19	43	9386-9389
ケイリン酸塩ガラスのイオン伝導特性	山田裕也, 岩崎秀, ZAGARZUSEM Khurelbaatar, JEEM Melbert, 小野円佳, 藤岡正弥, 小俣孝久, 西井準治	ガラスおよびフォトニクス材料討論会講演要旨集	2021	NOV	62		27-28
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Structural features of (Li,Na,K) PO3 mixed alkali metaphosphate glass for significant anisotropy	Endo, Jun; Inaba, Seiji; Homma, Osamu; Suzuki, Yoshikazu	JOURNAL OF THE AMERICAN CERAMIC SOCIETY	2022	JAN	105	1	217-224
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A new universal force-field for the Li2S-P2S5 system	Ariga, Shunsuke; Ohkubo, Takahiro; Urata, Shingo; Imamura, Yutaka; Taniguchi, Taketoshi	PHYSICAL CHEMISTRY CHEMICAL PHYSICS	2022	JAN	24	4	2567-2581
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Development of Machine-Learning Techniques for Time-of-Flight Secondary Ion Mass Spectrometry Spectral Analysis: Application for the Identification of Silane Coupling Agents in Multicomponent Films	Lang, Yusheng; Zhou, Lilin; Imamura, Yutaka	ANALYTICAL CHEMISTRY	2022	FEB	94	5	2546-2553
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Photo-on-Demand Phosgenation Reactions with Chloroform for Selective Syntheses of N-Substituted Ureas and Isocyanates	Muranaka Ryo, Liu Yue, Okada Itsuumi, Okazoe Takashi, Tsuda Akihiko	ACS Omega	2022	FEB	7	6	5584-5594
Suppression of Rayleigh Scattering in Silica Glass by Codoping Boron and Fluorine: Molecular Dynamics Simulations with Force-Matching and Neural Network Potentials	Urata, Shingo; Nakamura, Nobuhiro; Tada, Tomofumi; Tan, Aik Rui; Gomez-Bombarelli, Rafael; Hosono, Hideo	Journal of Physical Chemistry C	2022	FEB	126	4	2264-2275
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Glass etching with gaseous hydrogen fluoride: Rapid management of surface nano-roughness	Ono, Yoshitaka; Hayashi, Yasuo; Urashima, Shu-hei; Yui, Hiroharu	INTERNATIONAL JOURNAL OF APPLIED GLASS SCIENCE	2022	APR			
Speciation of tin ions in oxide glass containing iron oxide through solvent extraction and inductively coupled plasma atomic emission spectrometry after the decomposition utilizing ascorbic acid.	Saijo, Yoshitaka; Murata, Makiko; Kajihara, Takato; Hijiya, Hiroyuki; Suzuki, Yuichi; Akiyama, Ryoji; Shimizu, Masahiro; Shimotsuma, Yasuhiko; Miura, Kiyotaka	Analytical sciences : the international journal of the Japan Society for Analytical Chemistry	2022	APR	38	6	881-888
H2O2 adsorption and dissociation on various CeO2 (111) surface models: a first-principles study	Brugnoli, Luca; Urata, Shingo; Pedone, Alfonso	JOURNAL OF PHYSICS-CONDENSED MATTER	2022	APR	34	16	
Synthesis of Crystalline CF3-Rich Perfluoropolyethers from Hexafluoropropylene Oxide and (Trifluoromethyl) Trimethylsilane	Koyama, Minoru; Akiyama, Midori; Kashiwagi, Kimiaki; Nozaki, Kyoko; Okazoe, Takashi	MACRO MOLECULAR RAPID COMMUNICATIONS	2022	MAY	43	9	

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Adsorption characteristics of peptides on ω -functionalized self-assembled monolayers: a molecular dynamics study	Yadav, Hari O. S.; Kuo, An-Tsung; Urata, Shingo; Funahashi, Kosuke; Imamura, Yutaka; Shinoda, Wataru	Physical Chemistry Chemical Physics	2022	MAY	24		14805-14815
Synthesis of Crystalline CF ₃ -Rich Perfluoropolyethers from Hexafluoropropylene Oxide and (Trifluoromethyl) Trimethylsilane	Koyama Minoru, Akiyama Midori, Kashiwagi Kimiaki, Nozaki Kyoko, Okazoe Takashi, Okazoe Takashi	Macromolecular Rapid Communications	2022	MAY	43	9	e2200038
Theoretical estimation of dielectric loss of oxide glasses using nonequilibrium molecular dynamics simulations	Urata, Shingo; Hijiya, Hiroyuki; Niwano, Kazuhiko; Matsui, Jun	JOURNAL OF THE AMERICAN CERAMIC SOCIETY	2022	JUN	105	6	4200-4207
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