

Svemir Rudic

List of Publications by Year in descending order

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108
papers

4,021
citations

109321

35
h-index

133252

59
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108
all docs

108
docs citations

108
times ranked

4847
citing authors

#	ARTICLE	IF	CITATIONS
1	Selective Adsorption of Sulfur Dioxide in a Robust Metal-Organic Framework Material. <i>Advanced Materials</i> , 2016, 28, 8705-8711.	21.0	214
2	Identifying the Role of Terahertz Vibrations in Metal-Organic Frameworks: From Gate-Opening Phenomenon to Shear-Driven Structural Destabilization. <i>Physical Review Letters</i> , 2014, 113, 215502.	7.8	202
3	Confinement of Iodine Molecules into Triple-Helical Chains within Robust Metal-Organic Frameworks. <i>Journal of the American Chemical Society</i> , 2017, 139, 16289-16296.	13.7	199
4	Reversible coordinative binding and separation of sulfur dioxide in a robust metal-organic framework with open copper sites. <i>Nature Materials</i> , 2019, 18, 1358-1365.	27.5	171
5	Breaking the Limit of Lignin Monomer Production via Cleavage of Interunit Carbon-Carbon Linkages. <i>CheM</i> , 2019, 5, 1521-1536.	11.7	167
6	Inelastic neutron scattering study of reline: shedding light on the hydrogen bonding network of deep eutectic solvents. <i>Physical Chemistry Chemical Physics</i> , 2017, 19, 17998-18009.	2.8	132
7	Recent and future developments on TOSCA at ISIS. <i>Journal of Physics: Conference Series</i> , 2014, 554, 012003.	0.4	126
8	Inside PEF: Chain Conformation and Dynamics in Crystalline and Amorphous Domains. <i>Macromolecules</i> , 2018, 51, 3515-3526.	4.8	110
9	Paving the way for methane hydrate formation on metal-organic frameworks (MOFs). <i>Chemical Science</i> , 2016, 7, 3658-3666.	7.4	103
10	A comprehensive approach to investigate the structural and surface properties of activated carbons and related Pd-based catalysts. <i>Catalysis Science and Technology</i> , 2016, 6, 4910-4922.	4.1	96
11	Integration of mesopores and crystal defects in metal-organic frameworks via templated electrosynthesis. <i>Nature Communications</i> , 2019, 10, 4466.	12.8	90
12	The neutron guide upgrade of the TOSCA spectrometer. <i>Nuclear Instruments and Methods in Physics Research, Section A: Accelerators, Spectrometers, Detectors and Associated Equipment</i> , 2018, 896, 68-74.	1.6	84
13	Modulating supramolecular binding of carbon dioxide in a redox-active porous metal-organic framework. <i>Nature Communications</i> , 2017, 8, 14212.	12.8	75
14	Quantitative production of butenes from biomass-derived β -valerolactone catalysed by hetero-atomic MFI zeolite. <i>Nature Materials</i> , 2020, 19, 86-93.	27.5	74
15	Pore Distortion in a Metal-Organic Framework for Regulated Separation of Propane and Propylene. <i>Journal of the American Chemical Society</i> , 2021, 143, 19300-19305.	13.7	72
16	The dynamics of formation of HCl products from the reaction of Cl atoms with methanol, ethanol, and dimethyl ether. <i>Journal of Chemical Physics</i> , 2002, 117, 5692-5706.	3.0	69
17	On-the-fly ab initio trajectory calculations of the dynamics of Cl atom reactions with methane, ethane and methanol. <i>Journal of Chemical Physics</i> , 2004, 120, 186-198.	3.0	69
18	Graphitization of Activated Carbons: A Molecular-level Investigation by INS, DRIFT, XRD and Raman Techniques. <i>Physics Procedia</i> , 2016, 85, 20-26.	1.2	68

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19	High Ammonia Adsorption in MFM-300 Materials: Dynamics and Charge Transfer in Host-Guest Binding. <i>Journal of the American Chemical Society</i> , 2021, 143, 3153-3161.	13.7	67
20	Atomically Dispersed Copper Sites in a Metal-Organic Framework for Reduction of Nitrogen Dioxide. <i>Journal of the American Chemical Society</i> , 2021, 143, 10977-10985.	13.7	66
21	Detecting Molecular Rotational Dynamics Complementing the Low-Frequency Terahertz Vibrations in a Zirconium-Based Metal-Organic Framework. <i>Physical Review Letters</i> , 2017, 118, 255502.	7.8	60
22	Direct Evidence for Solid-like Hydrogen in a Nanoporous Carbon Hydrogen Storage Material at Supercritical Temperatures. <i>ACS Nano</i> , 2015, 9, 8249-8254.	14.6	57
23	Observation of Binding and Rotation of Methane and Hydrogen within a Functional Metal-Organic Framework. <i>Journal of the American Chemical Society</i> , 2016, 138, 9119-9127.	13.7	54
24	Structural dynamics of a metal-organic framework induced by CO ₂ migration in its non-uniform porous structure. <i>Nature Communications</i> , 2019, 10, 999.	12.8	54
25	Unexpected Cation Dynamics in the Low-Temperature Phase of Methylammonium Lead Iodide: The Need for Improved Models. <i>Journal of Physical Chemistry Letters</i> , 2016, 7, 4701-4709.	4.6	53
26	Predicting the reactivity of energetic materials: an <i>ab initio</i> multi-phonon approach. <i>Journal of Materials Chemistry A</i> , 2019, 7, 19539-19553.	10.3	52
27	Purification of Propylene and Ethylene by a Robust Metal-Organic Framework Mediated by Host-Guest Interactions. <i>Angewandte Chemie - International Edition</i> , 2021, 60, 15541-15547.	13.8	51
28	Host-guest selectivity in a series of isoreticular metal-organic frameworks: observation of acetylene-to-alkyne and carbon dioxide-to-amide interactions. <i>Chemical Science</i> , 2019, 10, 1098-1106.	7.4	47
29	Understanding the ZIF-L to ZIF-8 transformation from fundamentals to fully costed kilogram-scale production. <i>Communications Chemistry</i> , 2022, 5, .	4.5	45
30	Infrared laser spectroscopy of CH ₃ -HF in helium nanodroplets: The exit-channel complex of the F+CH ₄ reaction. <i>Journal of Chemical Physics</i> , 2006, 124, 084301.	3.0	44
31	Rotational distribution of the HCl products from the reaction of Cl(2P) atoms with methanol. <i>Chemical Physics Letters</i> , 2000, 332, 487-495.	2.6	43
32	Sources of Error and Uncertainty in the Use of Cavity Ring Down Spectroscopy to Measure Aerosol Optical Properties. <i>Aerosol Science and Technology</i> , 2011, 45, 1360-1375.	3.1	43
33	The product branching and dynamics of the reaction of chlorine atoms with methylamine. <i>Physical Chemistry Chemical Physics</i> , 2003, 5, 1205-1212.	2.8	41
34	Influence of Uncertainties in the Diameter and Refractive Index of Calibration Polystyrene Beads on the Retrieval of Aerosol Optical Properties Using Cavity Ring Down Spectroscopy. <i>Journal of Physical Chemistry A</i> , 2010, 114, 7077-7084.	2.5	41
35	Stereodynamics of Chlorine Atom Reactions with Organic Molecules. <i>Journal of Physical Chemistry A</i> , 2005, 109, 11093-11102.	2.5	39
36	Measurements of the wavelength dependent extinction of aerosols by cavity ring down spectroscopy. <i>Physical Chemistry Chemical Physics</i> , 2010, 12, 3914.	2.8	39

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37	Nuclear dynamics and phase polymorphism in solid formic acid. <i>Physical Chemistry Chemical Physics</i> , 2017, 19, 9064-9074.	2.8	33
38	Unusual flexibility of mesophase pitch-derived carbon materials: An approach to the synthesis of graphene. <i>Carbon</i> , 2017, 115, 539-545.	10.3	31
39	Carbohydrate hydration: heavy water complexes of α and β anomers of glucose, galactose, fucose and xylose. <i>Physical Chemistry Chemical Physics</i> , 2011, 13, 18671.	2.8	29
40	Emergence of glassy features in halomethane crystals. <i>Physical Review B</i> , 2019, 99, .	3.2	29
41	Nonlinear effects in pulsed cavity ringdown spectroscopy of lithium vapour. <i>Chemical Physics Letters</i> , 2000, 320, 613-622.	2.6	28
42	Hydrogen Bond Dynamics of Cellulose through Inelastic Neutron Scattering Spectroscopy. <i>Biomacromolecules</i> , 2018, 19, 1305-1313.	5.4	28
43	Guest-host interactions of nanoconfined anti-cancer drug in metal-organic framework exposed by terahertz dynamics. <i>Chemical Communications</i> , 2019, 55, 3868-3871.	4.1	27
44	Effect of pore geometry on ultra-densified hydrogen in microporous carbons. <i>Carbon</i> , 2021, 173, 968-979.	10.3	25
45	Guest-Controlled Incommensurate Modulation in a Meta-Rigid Metal-Organic Framework Material. <i>Journal of the American Chemical Society</i> , 2020, 142, 19189-19197.	13.7	24
46	Asymmetric Monomer, Amorphous Polymer? Structure-Property Relationships in 2,4-FDCA and 2,4-PEF. <i>Macromolecules</i> , 2020, 53, 1380-1387.	4.8	24
47	Direct Observation of Ammonia Storage in UiO-66 Incorporating Cu(II) Binding Sites. <i>Journal of the American Chemical Society</i> , 2022, 144, 8624-8632.	13.7	24
48	Heavy water hydration of mannose: the anomeric effect in solvation, laid bare. <i>Chemical Science</i> , 2011, 2, 1128.	7.4	23
49	Water dynamics in MCF-7 breast cancer cells: a neutron scattering descriptive study. <i>Scientific Reports</i> , 2019, 9, 8704.	3.3	23
50	Control of zeolite microenvironment for propene synthesis from methanol. <i>Nature Communications</i> , 2021, 12, 822.	12.8	23
51	Progress in the Characterization of the Surface Species in Activated Carbons by means of INS Spectroscopy Coupled with Detailed DFT Calculations. <i>Advances in Condensed Matter Physics</i> , 2015, 2015, 1-8.	1.1	22
52	Direct observation of supramolecular binding of light hydrocarbons in vanadium(III) and (IV) metal-organic framework materials. <i>Chemical Science</i> , 2018, 9, 3401-3408.	7.4	22
53	Detailed characterisation of the incident neutron beam on the TOSCA spectrometer. <i>Nuclear Instruments and Methods in Physics Research, Section A: Accelerators, Spectrometers, Detectors and Associated Equipment</i> , 2017, 870, 79-83.	1.6	22
54	The effect of surface chemistry on the performances of Pd-based catalysts supported on activated carbons. <i>Catalysis Science and Technology</i> , 2017, 7, 4162-4172.	4.1	21

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55	Vibrationally induced metallisation of the energetic azide $\text{N}_3\text{-NaN}$. <i>Physical Chemistry Chemical Physics</i> , 2018, 20, 29061-29069.	2.8	21
56	Infrared laser spectroscopy of the $\text{CH}_3\text{-HCN}$ radical complex stabilized in helium nanodroplets. <i>Journal of Chemical Physics</i> , 2006, 124, 104305.	3.0	20
57	Poly(4-styrene sulfonic acid)/bacterial cellulose membranes: Electrochemical performance in a single-chamber microbial fuel cell. <i>Bioresource Technology Reports</i> , 2020, 9, 100376.	2.7	20
58	Green Reconstruction of MIL-100 (Fe) in Water for High Crystallinity and Enhanced Guest Encapsulation. <i>ACS Sustainable Chemistry and Engineering</i> , 2020, 8, 8247-8255.	6.7	20
59	Conformational effects in sugar ions: spectroscopic investigations in the gas phase and in solution. <i>Chemical Science</i> , 2012, 3, 2307.	7.4	19
60	Monte carlo simulations of the TOSCA spectrometer: Assessment of current performance and future upgrades. <i>EPJ Web of Conferences</i> , 2015, 83, 03013.	0.3	19
61	Study of the $\text{CH}_3\text{-H}_2\text{O}$ radical complex stabilized in helium nanodroplets. <i>Physical Chemistry Chemical Physics</i> , 2009, 11, 5345.	2.8	17
62	Protonated sugars: vibrational spectroscopy and conformational structure of protonated O-methyl $\beta\text{-D-galactopyranoside}$. <i>Molecular Physics</i> , 2012, 110, 1609-1615.	1.7	17
63	A New Look into the Mode of Action of Metal-Based Anticancer Drugs. <i>Molecules</i> , 2020, 25, 246.	3.8	17
64	Water in Deep Eutectic Solvents: New Insights From Inelastic Neutron Scattering Spectroscopy. <i>Frontiers in Physics</i> , 2022, 10, .	2.1	17
65	Optical properties of micrometer size water droplets studied by cavity ringdown spectroscopy. <i>Applied Optics</i> , 2007, 46, 6142.	2.1	16
66	Influence of Solvent on Poly(2-(Dimethylamino)Ethyl Methacrylate) Dynamics in Polymer-Concentrated Mixtures: A Combined Neutron Scattering, Dielectric Spectroscopy, and Calorimetric Study. <i>Macromolecules</i> , 2015, 48, 6724-6735.	4.8	16
67	Neutronic developments on TOSCA and VESPA: Progress to date. <i>Physica B: Condensed Matter</i> , 2019, 562, 107-111.	2.7	16
68	OX-1 Metal-Organic Framework Nanosheets as Robust Hosts for Highly Active Catalytic Palladium Species. <i>ACS Sustainable Chemistry and Engineering</i> , 2019, 7, 5875-5885.	6.7	15
69	Measurement of the para-hydrogen concentration in the ISIS moderators using neutron transmission and thermal conductivity. <i>Nuclear Instruments and Methods in Physics Research, Section A: Accelerators, Spectrometers, Detectors and Associated Equipment</i> , 2018, 888, 88-95.	1.6	14
70	The TOSCA Spectrometer at ISIS: the Guide Upgrade and Beyond. <i>Journal of Physics: Conference Series</i> , 2018, 1021, 012029.	0.4	14
71	Predicting the impact sensitivity of a polymorphic high explosive: the curious case of FOX-7. <i>Chemical Communications</i> , 2021, 57, 11213-11216.	4.1	14
72	Origin of natural and magnetic field induced polar order in orthorhombic $\text{PrFe}_{1/2}\text{Cr}_{1/2}\text{O}_3$. <i>Physical Review B</i> , 2021, 104, .	3.2	14

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73	Confinement of poly(ethylene oxide) in the nanometer-scale pores of resins and carbon nanoparticles. <i>Soft Matter</i> , 2013, 9, 10960.	2.7	13
74	Intracellular water as a mediator of anticancer drug action. <i>International Reviews in Physical Chemistry</i> , 2020, 39, 67-81.	2.3	13
75	Intercalation and Confinement of Poly(ethylene oxide) in Porous Carbon Nanoparticles with Controlled Morphologies. <i>Macromolecules</i> , 2014, 47, 8729-8737.	4.8	12
76	Looking inside the pores of a MCM-41 based Mo heterogeneous styrene oxidation catalyst: an inelastic neutron scattering study. <i>Physical Chemistry Chemical Physics</i> , 2016, 18, 17272-17280.	2.8	12
77	CO ₂ Capture by Nickel Hydroxide Interstratified in the Nanolayered Space of a Synthetic Clay Mineral. <i>Journal of Physical Chemistry C</i> , 2020, 124, 26222-26231.	3.1	12
78	Understanding the Structure and Dynamics of Nanocellulose-Based Composites with Neutral and Ionic Poly(methacrylate) Derivatives Using Inelastic Neutron Scattering and DFT Calculations. <i>Molecules</i> , 2020, 25, 1689.	3.8	12
79	Direct Visualization of Supramolecular Binding and Separation of Light Hydrocarbons in MFM-300(In). <i>Chemistry of Materials</i> , 2022, 34, 5698-5705.	6.7	11
80	Determination of the scattering cross section of calcium using the VESUVIO spectrometer. <i>Nuclear Instruments and Methods in Physics Research, Section A: Accelerators, Spectrometers, Detectors and Associated Equipment</i> , 2019, 927, 443-450.	1.6	10
81	A HF Loaded Lewis Acidic Aluminium Chlorofluoride for Hydrofluorination Reactions. <i>Chemistry - A European Journal</i> , 2020, 26, 7314-7322.	3.3	10
82	Ammonia Storage in Hydrogen Bond-Rich Microporous Polymers. <i>ACS Applied Materials & Interfaces</i> , 2020, 12, 58161-58169.	8.0	9
83	Volatile Hydrogen Intermediates of CO ₂ Methanation by Inelastic Neutron Scattering. <i>Catalysts</i> , 2020, 10, 433.	3.5	9
84	Dynamics of hydrogen guests in ice XVII nanopores. <i>Physical Review Materials</i> , 2017, 1, .	2.4	9
85	Dynamics and Structure of Poly(ethylene oxide) Intercalated in the Nanopores of Resorcinol-Formaldehyde Resin Nanoparticles. <i>Macromolecules</i> , 2016, 49, 5704-5713.	4.8	8
86	Molecular Insights into Bulk and Porous P ₂ N ₄ -PTA Metal-Organic Polymers by Simultaneous Raman Spectroscopy and Inelastic Neutron Scattering. <i>European Journal of Inorganic Chemistry</i> , 2019, 2019, 1155-1161.	2.0	7
87	Spontaneous formation of an ordered interstratification upon Ni-exchange of Na-fluorohectorite. <i>Applied Clay Science</i> , 2020, 198, 105831.	5.2	7
88	Metallodrug-protein interaction probed by synchrotron terahertz and neutron scattering spectroscopy. <i>Biophysical Journal</i> , 2021, 120, 3070-3078.	0.5	7
89	Positional, isotopic mass and force constant disorder in molybdate glasses and their parent metal oxides as observed by neutron diffraction and Compton scattering. <i>Journal of Physics Communications</i> , 2020, 4, 095027.	1.2	7
90	A tale of two foils: ISIS TS-1 water moderators. <i>Journal of Physics: Conference Series</i> , 2018, 1021, 012039.	0.4	6

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91	Discovery of new neutron-moderating materials at ISIS Neutron and Muon Source. EPJ Web of Conferences, 2020, 239, 17008.	0.3	6
92	High capacity ammonia adsorption in a robust metal-organic framework mediated by reversible host-guest interactions. Chemical Communications, 2022, 58, 5753-5756.	4.1	6
93	A Python Algorithm to Analyze Inelastic Neutron Scattering Spectra Based on the γ -Scale Formalism. Journal of Chemical Theory and Computation, 2020, 16, 7671-7680.	5.3	5
94	Inelastic Neutron Scattering Investigation of MgCl_2 Nanoparticle-Based Ziegler-Natta Catalysts for Olefin Polymerization. ACS Applied Nano Materials, 2020, 3, 11118-11128.	5.0	5
95	Secondary relaxation in the terahertz range in 2-adamantanone from theory and experiments. Physical Review B, 2020, 101, .	3.2	5
96	Human hair: subtle change in the thioester groups dynamics observed by combining neutron scattering, X-ray diffraction and thermal analysis. European Physical Journal: Special Topics, 2020, 229, 2825-2832.	2.6	5
97	Hydrogen bond dynamics and conformational flexibility in antipsychotics. Physical Chemistry Chemical Physics, 2019, 21, 15463-15470.	2.8	4
98	Probing the relevance of MoO_2 nanoparticles TM synthesis on their catalytic activity by inelastic neutron scattering. Physical Chemistry Chemical Physics, 2020, 22, 896-904.	2.8	4
99	Density of Phonon States in Cubic Ice Ic. Journal of Physical Chemistry C, 2021, 125, 23533-23538.	3.1	4
100	Interplay between Local Structure and Nuclear Dynamics in Tungstic Acid: A Neutron Scattering Study. Journal of Physical Chemistry C, 2021, 125, 23864-23879.	3.1	4
101	Spectroscopic Signatures of Hydrogen-Bonding Motifs in Protonic Ionic Liquid Systems: Insights from Diethylammonium Nitrate in the Solid State. Journal of Physical Chemistry C, 2021, 125, 24463-24476.	3.1	4
102	Crystal Analyzers for Indirect-Geometry Broadband Neutron Spectrometers: Adding Reality to Idealized Design. Journal of Surface Investigation, 2020, 14, S242-S250.	0.5	3
103	Understanding the effect of lattice polarisability on the electrochemical properties of lithium tetrahaloaluminates, LiAlX_4 ($\text{X} = \text{Cl}, \text{Br}, \text{I}$). Journal of Materials Chemistry A, 2020, .	10.3	3
104	Spin isomers in the ISIS TS1 cryogenic hydrogen moderator. Journal of Physics: Conference Series, 2018, 1021, 012057.	0.4	2
105	Robust measurement of para-ortho H_2 ratios to characterise the ISIS hydrogen moderators. Journal of Physics: Conference Series, 2018, 1021, 012055.	0.4	2
106	Hydrogen Detection Limits and Instrument Sensitivity of High-Resolution Broadband Neutron Spectrometers. Analytical Chemistry, 2022, 94, 5023-5028.	6.5	2
107	Cryogenic sample environment on TOSCA. Journal of Physics: Conference Series, 2014, 554, 012007.	0.4	1
108	Spectroscopic Identification of Disordered Molecular Cations in Defect Perovskite-like $\text{Aln}(\text{HCO}_2)(\text{C}_2\text{O}_4)_{1.5}$ ($\text{Ln} = \text{Tb}, \text{Er}$) Phases. European Journal of Inorganic Chemistry, 2021, 2021, 3806.	2.0	1