Svemir Rudic

List of Publications by Year in descending order

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108 4,021 papers citations

35 h-index 59 g-index

108 all docs 108 docs citations 108 times ranked 4847 citing authors

#	Article	IF	CITATIONS
1	Water in Deep Eutectic Solvents: New Insights From Inelastic Neutron Scattering Spectroscopy. Frontiers in Physics, 2022, 10, .	1.0	17
2	Understanding the ZIF-L to ZIF-8 transformation from fundamentals to fully costed kilogram-scale production. Communications Chemistry, 2022, 5, .	2.0	45
3	Hydrogen Detection Limits and Instrument Sensitivity of High-Resolution Broadband Neutron Spectrometers. Analytical Chemistry, 2022, 94, 5023-5028.	3.2	2
4	High capacity ammonia adsorption in a robust metal–organic framework mediated by reversible host–guest interactions. Chemical Communications, 2022, 58, 5753-5756.	2.2	6
5	Direct Observation of Ammonia Storage in UiO-66 Incorporating Cu(II) Binding Sites. Journal of the American Chemical Society, 2022, 144, 8624-8632.	6.6	24
6	Direct Visualization of Supramolecular Binding and Separation of Light Hydrocarbons in MFM-300(In). Chemistry of Materials, 2022, 34, 5698-5705.	3.2	11
7	Effect of pore geometry on ultra-densified hydrogen in microporous carbons. Carbon, 2021, 173, 968-979.	5.4	25
8	Predicting the impact sensitivity of a polymorphic high explosive: the curious case of FOX-7. Chemical Communications, 2021, 57, 11213-11216.	2.2	14
9	High Ammonia Adsorption in MFM-300 Materials: Dynamics and Charge Transfer in Host–Guest Binding. Journal of the American Chemical Society, 2021, 143, 3153-3161.	6.6	67
10	Control of zeolite microenvironment for propene synthesis from methanol. Nature Communications, 2021, 12, 822.	5.8	23
11	Purification of Propylene and Ethylene by a Robust Metal–Organic Framework Mediated by Host–Guest Interactions. Angewandte Chemie - International Edition, 2021, 60, 15541-15547.	7.2	51
12	Spectroscopic Identification of Disordered Molecular Cations in Defect Perovskiteâ€like ALn(HCO2)(C2O4)1.5 (Ln = Tbâ€Er) Phases. European Journal of Inorganic Chemistry, 2021, 2021, 3806.	1.0	1
13	Atomically Dispersed Copper Sites in a Metal–Organic Framework for Reduction of Nitrogen Dioxide. Journal of the American Chemical Society, 2021, 143, 10977-10985.	6.6	66
14	Origin of natural and magnetic field induced polar order in orthorhombic PrFe1/2Cr1/2O3. Physical Review B, 2021, 104, .	1.1	14
15	Metallodrug-protein interaction probed by synchrotron terahertz and neutron scattering spectroscopy. Biophysical Journal, 2021, 120, 3070-3078.	0.2	7
16	Density of Phonon States in Cubic Ice Ic. Journal of Physical Chemistry C, 2021, 125, 23533-23538.	1.5	4
17	Interplay between Local Structure and Nuclear Dynamics in Tungstic Acid: A Neutron Scattering Study. Journal of Physical Chemistry C, 2021, 125, 23864-23879.	1.5	4
18	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.	1.5	4

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19	Pore Distortion in a Metal–Organic Framework for Regulated Separation of Propane and Propylene. Journal of the American Chemical Society, 2021, 143, 19300-19305.	6.6	72
20	Probing the relevance of MoO ₂ nanoparticles' synthesis on their catalytic activity by inelastic neutron scattering. Physical Chemistry Chemical Physics, 2020, 22, 896-904.	1.3	4
21	Quantitative production of butenes from biomass-derived \hat{I}^3 -valerolactone catalysed by hetero-atomic MFI zeolite. Nature Materials, 2020, 19, 86-93.	13.3	74
22	Poly(4-styrene sulfonic acid)/bacterial cellulose membranes: Electrochemical performance in a single-chamber microbial fuel cell. Bioresource Technology Reports, 2020, 9, 100376.	1.5	20
23	Discovery of new neutron-moderating materials at ISIS Neutron and Muon Source. EPJ Web of Conferences, 2020, 239, 17008.	0.1	6
24	CO ₂ Capture by Nickel Hydroxide Interstratified in the Nanolayered Space of a Synthetic Clay Mineral. Journal of Physical Chemistry C, 2020, 124, 26222-26231.	1.5	12
25	A Python Algorithm to Analyze Inelastic Neutron Scattering Spectra Based on the y-Scale Formalism. Journal of Chemical Theory and Computation, 2020, 16, 7671-7680.	2.3	5
26	Inelastic Neutron Scattering Investigation of MgCl ₂ Nanoparticle-Based Ziegler–Natta Catalysts for Olefin Polymerization. ACS Applied Nano Materials, 2020, 3, 11118-11128.	2.4	5
27	Guest-Controlled Incommensurate Modulation in a Meta-Rigid Metal–Organic Framework Material. Journal of the American Chemical Society, 2020, 142, 19189-19197.	6.6	24
28	Ammonia Storage in Hydrogen Bond-Rich Microporous Polymers. ACS Applied Materials & Samp; Interfaces, 2020, 12, 58161-58169.	4.0	9
29	Spontaneous formation of an ordered interstratification upon Ni-exchange of Na-fluorohectorite. Applied Clay Science, 2020, 198, 105831.	2.6	7
30	Green Reconstruction of MIL-100 (Fe) in Water for High Crystallinity and Enhanced Guest Encapsulation. ACS Sustainable Chemistry and Engineering, 2020, 8, 8247-8255.	3.2	20
31	Secondary relaxation in the terahertz range in 2-adamantanone from theory and experiments. Physical Review B, 2020, 101, .	1.1	5
32	A New Look into the Mode of Action of Metal-Based Anticancer Drugs. Molecules, 2020, 25, 246.	1.7	17
33	Intracellular water as a mediator of anticancer drug action. International Reviews in Physical Chemistry, 2020, 39, 67-81.	0.9	13
34	Asymmetric Monomer, Amorphous Polymer? Structure–Property Relationships in 2,4-FDCA and 2,4-PEF. Macromolecules, 2020, 53, 1380-1387.	2.2	24
35	Understanding the Structure and Dynamics of Nanocellulose-Based Composites with Neutral and Ionic Poly(methacrylate) Derivatives Using Inelastic Neutron Scattering and DFT Calculations. Molecules, 2020, 25, 1689 .	1.7	12
36	Volatile Hydrogen Intermediates of CO2 Methanation by Inelastic Neutron Scattering. Catalysts, 2020, 10, 433.	1.6	9

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37	A HF Loaded Lewisâ€Acidic Aluminium Chlorofluoride for Hydrofluorination Reactions. Chemistry - A European Journal, 2020, 26, 7314-7322.	1.7	10
38	Positional, isotopic mass and force constant disorder in molybdate glasses and their parent metal oxides as observed by neutron diffraction and Compton scattering. Journal of Physics Communications, 2020, 4, 095027.	0.5	7
39	Crystal Analyzers for Indirect-Geometry Broadband Neutron Spectrometers: Adding Reality to Idealized Design. Journal of Surface Investigation, 2020, 14, S242-S250.	0.1	3
40	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.	1.2	5
41	Predicting the reactivity of energetic materials: an <i>ab initio</i> multi-phonon approach. Journal of Materials Chemistry A, 2019, 7, 19539-19553.	5.2	52
42	Hydrogen bond dynamics and conformational flexibility in antipsychotics. Physical Chemistry Chemical Physics, 2019, 21, 15463-15470.	1.3	4
43	Host–guest selectivity in a series of isoreticular metal–organic frameworks: observation of acetylene-to-alkyne and carbon dioxide-to-amide interactions. Chemical Science, 2019, 10, 1098-1106.	3.7	47
44	Water dynamics in MCF-7 breast cancer cells: a neutron scattering descriptive study. Scientific Reports, 2019, 9, 8704.	1.6	23
45	Breaking the Limit of Lignin Monomer Production via Cleavage of Interunit Carbon–Carbon Linkages. CheM, 2019, 5, 1521-1536.	5.8	167
46	Determination of the scattering cross section of calcium using the VESUVIO spectrometer. Nuclear Instruments and Methods in Physics Research, Section A: Accelerators, Spectrometers, Detectors and Associated Equipment, 2019, 927, 443-450.	0.7	10
47	Molecular Insights into Bulk and Porous ΰ ² <i>P,N</i> â€PTA Metalâ€Organic Polymers by Simultaneous Raman Spectroscopy and Inelastic Neutron Scattering. European Journal of Inorganic Chemistry, 2019, 2019, 1155-1161.	1.0	7
48	Neutronic developments on TOSCA and VESPA: Progress to date. Physica B: Condensed Matter, 2019, 562, 107-111.	1.3	16
49	Structural dynamics of a metal–organic framework induced by CO2 migration in its non-uniform porous structure. Nature Communications, 2019, 10, 999.	5.8	54
50	Guest–host interactions of nanoconfined anti-cancer drug in metal–organic framework exposed by terahertz dynamics. Chemical Communications, 2019, 55, 3868-3871.	2.2	27
51	OX-1 Metal–Organic Framework Nanosheets as Robust Hosts for Highly Active Catalytic Palladium Species. ACS Sustainable Chemistry and Engineering, 2019, 7, 5875-5885.	3.2	15
52	Integration of mesopores and crystal defects in metal-organic frameworks via templated electrosynthesis. Nature Communications, 2019, 10, 4466.	5 . 8	90
53	Reversible coordinative binding and separation of sulfur dioxide in a robust metal–organic framework with open copper sites. Nature Materials, 2019, 18, 1358-1365.	13.3	171
54	Emergence of glassy features in halomethane crystals. Physical Review B, 2019, 99, .	1.1	29

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55	Direct observation of supramolecular binding of light hydrocarbons in vanadium(<scp>iii</scp>) and (<scp>iv</scp>) metal–organic framework materials. Chemical Science, 2018, 9, 3401-3408.	3.7	22
56	The neutron guide upgrade of the TOSCA spectrometer. Nuclear Instruments and Methods in Physics Research, Section A: Accelerators, Spectrometers, Detectors and Associated Equipment, 2018, 896, 68-74.	0.7	84
57	Measurement of the para-hydrogen concentration in the ISIS moderators using neutron transmission and thermal conductivity. Nuclear Instruments and Methods in Physics Research, Section A: Accelerators, Spectrometers, Detectors and Associated Equipment, 2018, 888, 88-95.	0.7	14
58	Inside PEF: Chain Conformation and Dynamics in Crystalline and Amorphous Domains. Macromolecules, 2018, 51, 3515-3526.	2.2	110
59	Hydrogen Bond Dynamics of Cellulose through Inelastic Neutron Scattering Spectroscopy. Biomacromolecules, 2018, 19, 1305-1313.	2.6	28
60	Spin isomers in the ISIS TS1 cryogenic hydrogen moderator. Journal of Physics: Conference Series, 2018, 1021, 012057.	0.3	2
61	A tale of two foils: ISIS TS-1 water moderators. Journal of Physics: Conference Series, 2018, 1021, 012039.	0.3	6
62	Vibrationally induced metallisation of the energetic azide \hat{l} ±-NaN ₃ . Physical Chemistry Chemical Physics, 2018, 20, 29061-29069.	1.3	21
63	The TOSCA Spectrometer at ISIS: the Guide Upgrade and Beyond. Journal of Physics: Conference Series, 2018, 1021, 012029.	0.3	14
64	Robust measurement of para-ortho H ₂ ratios to characterise the ISIS hydrogen moderators. Journal of Physics: Conference Series, 2018, 1021, 012055.	0.3	2
65	Unusual flexibility of mesophase pitch-derived carbon materials: An approach to the synthesis of graphene. Carbon, 2017, 115, 539-545.	5.4	31
66	Modulating supramolecular binding of carbon dioxide in a redox-active porous metal-organic framework. Nature Communications, 2017, 8, 14212.	5.8	75
67	Inelastic neutron scattering study of reline: shedding light on the hydrogen bonding network of deep eutectic solvents. Physical Chemistry Chemical Physics, 2017, 19, 17998-18009.	1.3	132
68	Nuclear dynamics and phase polymorphism in solid formic acid. Physical Chemistry Chemical Physics, 2017, 19, 9064-9074.	1.3	33
69	Confinement of Iodine Molecules into Triple-Helical Chains within Robust Metal–Organic Frameworks. Journal of the American Chemical Society, 2017, 139, 16289-16296.	6.6	199
70	The effect of surface chemistry on the performances of Pd-based catalysts supported on activated carbons. Catalysis Science and Technology, 2017, 7, 4162-4172.	2.1	21
71	Detecting Molecular Rotational Dynamics Complementing the Low-Frequency Terahertz Vibrations in a Zirconium-Based Metal-Organic Framework. Physical Review Letters, 2017, 118, 255502.	2.9	60
72	Detailed characterisation of the incident neutron beam on the TOSCA spectrometer. Nuclear Instruments and Methods in Physics Research, Section A: Accelerators, Spectrometers, Detectors and Associated Equipment, 2017, 870, 79-83.	0.7	22

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73	Dynamics of hydrogen guests in ice XVII nanopores. Physical Review Materials, 2017, 1, .	0.9	9
74	Graphitization of Activated Carbons: A Molecular-level Investigation by INS, DRIFT, XRD and Raman Techniques. Physics Procedia, 2016, 85, 20-26.	1.2	68
75	Looking inside the pores of a MCM-41 based Mo heterogeneous styrene oxidation catalyst: an inelastic neutron scattering study. Physical Chemistry Chemical Physics, 2016, 18, 17272-17280.	1.3	12
76	Dynamics and Structure of Poly(ethylene oxide) Intercalated in the Nanopores of Resorcinol–Formaldehyde Resin Nanoparticles. Macromolecules, 2016, 49, 5704-5713.	2.2	8
77	Selective Adsorption of Sulfur Dioxide in a Robust Metal–Organic Framework Material. Advanced Materials, 2016, 28, 8705-8711.	11.1	214
78	Observation of Binding and Rotation of Methane and Hydrogen within a Functional Metal–Organic Framework. Journal of the American Chemical Society, 2016, 138, 9119-9127.	6.6	54
79	A comprehensive approach to investigate the structural and surface properties of activated carbons and related Pd-based catalysts. Catalysis Science and Technology, 2016, 6, 4910-4922.	2.1	96
80	Unexpected Cation Dynamics in the Low-Temperature Phase of Methylammonium Lead Iodide: The Need for Improved Models. Journal of Physical Chemistry Letters, 2016, 7, 4701-4709.	2.1	53
81	Paving the way for methane hydrate formation on metal–organic frameworks (MOFs). Chemical Science, 2016, 7, 3658-3666.	3.7	103
82	Monte carlo simulations of the TOSCA spectrometer: Assessment of current performance and future upgrades. EPJ Web of Conferences, 2015, 83, 03013.	0.1	19
83	Progress in the Characterization of the Surface Species in Activated Carbons by means of INS Spectroscopy Coupled with Detailed DFT Calculations. Advances in Condensed Matter Physics, 2015, 2015, 1-8.	0.4	22
84	Direct Evidence for Solid-like Hydrogen in a Nanoporous Carbon Hydrogen Storage Material at Supercritical Temperatures. ACS Nano, 2015, 9, 8249-8254.	7.3	57
85	Influence of Solvent on Poly(2-(Dimethylamino)Ethyl Methacrylate) Dynamics in Polymer-Concentrated Mixtures: A Combined Neutron Scattering, Dielectric Spectroscopy, and Calorimetric Study. Macromolecules, 2015, 48, 6724-6735.	2.2	16
86	Intercalation and Confinement of Poly(ethylene oxide) in Porous Carbon Nanoparticles with Controlled Morphologies. Macromolecules, 2014, 47, 8729-8737.	2.2	12
87	Identifying the Role of Terahertz Vibrations in Metal-Organic Frameworks: From Gate-Opening Phenomenon to Shear-Driven Structural Destabilization. Physical Review Letters, 2014, 113, 215502.	2.9	202
88	Recent and future developments on TOSCA at ISIS. Journal of Physics: Conference Series, 2014, 554, 012003.	0.3	126
89	Cryogenic sample environment on TOSCA. Journal of Physics: Conference Series, 2014, 554, 012007.	0.3	1
90	Confinement of poly(ethylene oxide) in the nanometer-scale pores of resins and carbon nanoparticles. Soft Matter, 2013, 9, 10960.	1.2	13

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91	Protonated sugars: vibrational spectroscopy and conformational structure of protonatedO-methyl α-D-galactopyranoside. Molecular Physics, 2012, 110, 1609-1615.	0.8	17
92	Conformational effects in sugar ions: spectroscopic investigations in the gas phase and in solution. Chemical Science, 2012, 3, 2307.	3.7	19
93	Carbohydrate hydration: heavy water complexes of \hat{l}_{\pm} and \hat{l}_{-}^2 anomers of glucose, galactose, fucose and xylose. Physical Chemistry Chemical Physics, 2011, 13, 18671.	1.3	29
94	Heavy water hydration of mannose: the anomeric effect in solvation, laid bare. Chemical Science, 2011, 2, 1128.	3.7	23
95	Sources of Error and Uncertainty in the Use of Cavity Ring Down Spectroscopy to Measure Aerosol Optical Properties. Aerosol Science and Technology, 2011, 45, 1360-1375.	1.5	43
96	Measurements of the wavelength dependent extinction of aerosols by cavity ring down spectroscopy. Physical Chemistry Chemical Physics, 2010, 12, 3914.	1.3	39
97	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. Journal of Physical Chemistry A, 2010, 114, 7077-7084.	1.1	41
98	Study of the CH3 \hat{a}^{-} H2O radical complex stabilized in helium nanodroplets. Physical Chemistry Chemical Physics, 2009, 11, 5345.	1.3	17
99	Optical properties of micrometer size water droplets studied by cavity ringdown spectroscopy. Applied Optics, 2007, 46, 6142.	2.1	16
100	Infrared laser spectroscopy of the CH3–HCN radical complex stabilized in helium nanodroplets. Journal of Chemical Physics, 2006, 124, 104305.	1.2	20
101	Infrared laser spectroscopy of CH3â< HF in helium nanodroplets: The exit-channel complex of the F+CH4 reaction. Journal of Chemical Physics, 2006, 124, 084301.	1.2	44
102	Stereodynamics of Chlorine Atom Reactions with Organic Molecules. Journal of Physical Chemistry A, 2005, 109, 11093-11102.	1,1	39
103	On-the-flyab initiotrajectory calculations of the dynamics of Cl atom reactions with methane, ethane and methanol. Journal of Chemical Physics, 2004, 120, 186-198.	1.2	69
104	The product branching and dynamics of the reaction of chlorine atoms with methylamine. Physical Chemistry Chemical Physics, 2003, 5, 1205-1212.	1.3	41
105	The dynamics of formation of HCl products from the reaction of Cl atoms with methanol, ethanol, and dimethyl ether. Journal of Chemical Physics, 2002, 117, 5692-5706.	1.2	69
106	Nonlinear effects in pulsed cavity ringdown spectroscopy of lithium vapour. Chemical Physics Letters, 2000, 320, 613-622.	1.2	28
107	Rotational distribution of the HCl products from the reaction of Cl(2P) atoms with methanol. Chemical Physics Letters, 2000, 332, 487-495.	1.2	43
108	Understanding the effect of lattice polarisability on the electrochemical properties of lithium tetrahaloaluminates, LiAl <i>X</i> $XXX<$	5.2	3