

StÃ©phane Rols

List of Publications by Year in descending order

Source: <https://exaly.com/author-pdf/7129792/publications.pdf>

Version: 2024-02-01

150
papers

4,102
citations

117453

34
h-index

138251

58
g-index

150
all docs

150
docs citations

150
times ranked

4912
citing authors

#	ARTICLE	IF	CITATIONS
1	Resonant Raman study of the structure and electronic properties of single-wall carbon nanotubes. Chemical Physics Letters, 2000, 316, 186-190.	1.2	226
2	Design of Single-Molecule Magnets: Insufficiency of the Anisotropy Barrier as the Sole Criterion. Inorganic Chemistry, 2015, 54, 7600-7606.	1.9	191
3	The dipolar endofullerene HF@C60. Nature Chemistry, 2016, 8, 953-957.	6.6	167
4	Modifying the properties of 4f single-ion magnets by peripheral ligand functionalisation. Chemical Science, 2014, 5, 1650-1660.	3.7	159
5	Quantum rotation of <i>ortho</i> and <i>para</i> -water encapsulated in a fullerene cage. Proceedings of the National Academy of Sciences of the United States of America, 2012, 109, 12894-12898.	3.3	135
6	Phonons in single wall carbon nanotube bundles. Carbon, 2002, 40, 1697-1714.	5.4	124
7	Diffraction by finite-size crystalline bundles of single wall nanotubes. European Physical Journal B, 1999, 10, 263-270.	0.6	123
8	New Insight into the Vibrational Behavior of Nickel Hydroxide and Oxyhydroxide Using Inelastic Neutron Scattering, Far/Mid-Infrared and Raman Spectroscopies. Journal of Physical Chemistry C, 2008, 112, 2193-2201.	1.5	119
9	Diameter distribution of single wall carbon nanotubes in nanobundles. European Physical Journal B, 2000, 18, 201-205.	0.6	109
10	Polygonization of single-wall carbon nanotube bundles under high pressure. Physical Review B, 2001, 64, .	1.1	87
11	Chemical tunnel-splitting-engineering in a dysprosium-based molecular nanomagnet. Nature Communications, 2018, 9, 1292.	5.8	81
12	Phonon Density of States of Single-Wall Carbon Nanotubes. Physical Review Letters, 2000, 85, 5222-5225.	2.9	73
13	Nonresonant Raman spectrum in infinite and finite single-wall carbon nanotubes. Physical Review B, 2002, 66, .	1.1	72
14	Ab initio lattice dynamics simulations and inelastic neutron scattering spectra for studying phonons in BaFe_2As_2 . Effect of structural phase transition, structural relaxation, and magnetic ordering. Physical Review B, 2009, 79, .	2.1	64
15	Connection between Boson Peak and Elastic Properties in Silicate Glasses. Physical Review Letters, 2009, 102, 195502.	2.9	61
16	Quantum Translator-Rotator: Inelastic Neutron Scattering of Dihydrogen Molecules Trapped inside Anisotropic Fullerene Cages. Physical Review Letters, 2009, 102, 013001.	2.9	61
17	Symmetry-breaking in the endofullerene $\text{H}_2\text{O}@C_{60}$ revealed in the quantum dynamics of ortho and para-water: a neutron scattering investigation. Physical Chemistry Chemical Physics, 2014, 16, 21330-21339.	1.3	59
18	Inelastic neutron scattering of a quantum translator-rotator encapsulated in a closed fullerene cage: Isotope effects and translation-rotation coupling in $\text{H}_2\text{O}@C_{60}$. Physical Review B, 2010, 82, .	1.1	57

#	ARTICLE	IF	CITATIONS
19	Neutron diffraction and numerical modelling investigation of methane adsorption on bundles of carbon nanotubes. Chemical Physics, 2003, 293, 217-230.	0.9	56
20	Soft-phonon mediated structural phase transition in GeTe. Physical Review B, 2014, 89, .	1.1	56
21	Argon adsorption in open-ended single-wall carbon nanotubes. Physical Review B, 2005, 71, .	1.1	55
22	Inelastic neutron scattering and lattice-dynamical calculations of BaFe ₂ As ₂ . Physical Review B, 2008, 78, .	1.1	54
23	On the diffraction pattern of C ₆₀ peapods. European Physical Journal B, 2004, 42, 31-45.	0.6	51
24	Excitation energy dependence of the Raman spectrum of single-walled carbon nanotubes. Chemical Physics Letters, 2000, 320, 441-447.	1.2	49
25	Inelastic neutron scattering investigations of the quantum molecular dynamics of a H ₂ O molecule entrapped inside a fullerene cage. Physical Review B, 2012, 85, .	1.1	45
26	Orientation of single-walled carbon nanotubes by uniaxial pressure. Journal of Applied Physics, 2003, 93, 1769-1773.	1.1	43
27	Vibrations and hydrogen bonding in porphycene. Physical Chemistry Chemical Physics, 2012, 14, 5489.	1.3	41
28	Structural determination of iodine localization in single-walled carbon nanotube bundles by diffraction methods. Physical Review B, 2004, 69, .	1.1	40
29	How Confinement Affects the Dynamics of C ₆₀ in Carbon Nanopeapods. Physical Review Letters, 2008, 101, 065507.	2.9	40
30	Specific Heat of (GeTe) _x (Sb ₂ Te ₃) _{1-x} Phase-Change Materials: The Impact of Disorder and Anharmonicity. Chemistry of Materials, 2014, 26, 2307-2312.	3.2	40
31	Monitoring molecular motion in nano-porous solids. Comptes Rendus Physique, 2007, 8, 777-788.	0.3	36
32	Diameter dependence of Raman intensities for single-wall carbon nanotubes. Physical Review B, 2001, 63, .	1.1	35
33	Phase transitions and thermodynamic properties of yttria, Y ₂ O ₃ : Inelastic neutron scattering shell model and first-principles calculations. Physical Review B, 2011, 84, .	1.1	35
34	X-ray Scattering Determination of the Structure of Water during Carbon Nanotube Filling. Nano Letters, 2013, 13, 1751-1756.	4.5	35
35	Communication: High-frequency acoustic excitations and boson peak in glasses: A study of their temperature dependence. Journal of Chemical Physics, 2010, 133, 041101.	1.2	34
36	Localised Ag ⁺ vibrations at the origin of ultralow thermal conductivity in layered thermoelectric AgCrSe ₂ . Scientific Reports, 2016, 6, 23415.	1.6	34

#	ARTICLE	IF	CITATIONS
37	Quantum rotation and translation of hydrogen molecules encapsulated inside C ₆₀ : temperature dependence of inelastic neutron scattering spectra. Philosophical Transactions Series A, Mathematical, Physical, and Engineering Sciences, 2013, 371, 20110627.	1.6	32
38	Local Structure, Dynamics, and the Mechanisms of Oxide Ionic Conduction in Bi ₂₆ Mo ₁₀ O ₆₉ . Chemistry of Materials, 2012, 24, 4607-4614.	3.2	30
39	Phonons, nature of bonding, and their relation to anomalous thermal expansion behavior of M ₂ O (M) Tj ETQq1 1 0,784314 rgBT /Over	1.1	30
40	Quantum fluctuations and the magnetic ground state of Ce Physical Review B, 2010, 81, .	1.1	29
41	Lattice dynamics of rhenium trioxide from the quasiharmonic approximation. Physical Review B, 2010, 82, .	1.1	29
42	Structural properties of carbon peapods under extreme conditions studied using in situ x-ray diffraction. Physical Review B, 2006, 74, .	1.1	28
43	Discriminated structural behaviour of C ₆₀ and C ₇₀ peapods under extreme conditions. Europhysics Letters, 2007, 79, 56003.	0.7	28
44	Anomalous vibrational dynamics in the MgZn Zn	1.1	28
45	Synthesis and Properties of Open Fullerenes Encapsulating Ammonia and Methane. ChemPhysChem, 2018, 19, 266-276.	1.0	28
46	Confirming a Predicted Selection Rule in Inelastic Neutron Scattering Spectroscopy: The Quantum Translator-Rotator H_2 Entrapped Inside C_{60}	2.9	27
47	Tracking the Hydrogen Motion in Defective Graphene. Journal of Physical Chemistry C, 2014, 118, 7110-7116.	1.5	26
48	Lattice dynamics and thermal expansion behavior in the metal cyanides M_2CN_2	1.1	26
49	Symmetry-breaking in the $H_2@C_{60}$ endofullerene revealed by inelastic neutron scattering at low temperature. Physical Chemistry Chemical Physics, 2016, 18, 1998-2005.	1.3	25
50	Effect of pore geometry on ultra-densified hydrogen in microporous carbons. Carbon, 2021, 173, 968-979.	5.4	25
51	Magnetic lattice dynamics of the oxygen-free FeAs pnictides: how sensitive are phonons to magnetic ordering?. Journal of Physics Condensed Matter, 2010, 22, 315701.	0.7	24
52	Direct Determination of the Base-Pair Force Constant of DNA from the Acoustic Phonon Dispersion of the Double Helix. Physical Review Letters, 2011, 107, 088102.	2.9	24
53	Low-frequency excitations of C ₆₀ chains inserted inside single-walled carbon nanotubes. Physical Review B, 2005, 71, .	1.1	23
54	Phonon dynamics in Sr _{0.6} K _{0.4} Fe ₂ As ₂ and Ca _{0.6} Na _{0.4} Fe ₂ As ₂ from neutron scattering and lattice-dynamical calculations. Physical Review B, 2008, 78, .	1.1	23

#	ARTICLE	IF	CITATIONS
55	Calculation of Raman-active modes in linear and zigzag phases of fullerene peapods. <i>Physical Review B</i> , 2006, 74, .	1.1	22
56	X-ray diffraction as a tool for the determination of the structure of double-walled carbon nanotube batches. <i>Physical Review B</i> , 2009, 79, .	1.1	22
57	Comment on "Effect of the Growth Temperature on the Diameter Distribution and Chirality of Single-Wall Carbon Nanotubes". <i>Physical Review Letters</i> , 1998, 81, 4780-4780.	2.9	20
58	Neutron scattering studies of the structure and dynamics of nanobundles of single-wall carbon nanotubes. <i>Applied Physics A: Materials Science and Processing</i> , 1999, 69, 591-596.	1.1	20
59	Effects of magnetic doping and temperature dependence of phonon dynamics in $\text{CaFe}_{1-x}\text{Co}_x\text{AsF}$ compounds ($x=0, 0.06, \text{ and } 0.12$). <i>Physical Review B</i> , 2009, 79, .	1.1	20
60	Hydrogen on graphene investigated by inelastic neutron scattering. <i>Journal of Physics: Conference Series</i> , 2014, 554, 012009.	0.3	20
61	Anomalous lattice behavior of vanadium pentaoxide (V_2O_5): X-ray diffraction, inelastic neutron scattering and ab initio lattice dynamics. <i>Physical Chemistry Chemical Physics</i> , 2017, 19, 17967-17984.	1.3	20
62	Size-Dependent Phase Transition of Diamond to Graphite at High Pressures. <i>Journal of Physical Chemistry C</i> , 2007, 111, 12918-12925.	1.5	18
63	Ordering and dynamics of the central tetrahedron in the $1/1 \text{ Zn}_{26}\text{Sc}$ periodic approximant to quasicrystal. <i>Journal of Physics Condensed Matter</i> , 2012, 24, 415403.	0.7	18
64	Possible coupling between magnons and phonons in multiferroic $\text{CaMn}_7\text{O}_{12}$. <i>Physical Review B</i> , 2014, 90, .	1.1	18
65	Phonon dynamics and inelastic neutron scattering of sodium niobate. <i>Physical Review B</i> , 2014, 89, .	1.1	18
66	Density of states in solid deuterium: Inelastic neutron scattering study. <i>Physical Review B</i> , 2009, 80, .	1.1	17
67	Phonon spectra in CaFe_2As_2 and $\text{Ca}_{0.6}\text{Na}_{0.4}\text{Fe}_2\text{As}_2$: Measurement of the pressure and temperature dependence and comparison with ab initio and shell model calculations. <i>Physical Review B</i> , 2009, 79, .	1.1	17
68	Spin-phonon coupling in $\text{K}_{0.8}\text{FeSe}$. <i>Physical Review B</i> , 2016, 93, 040401.	1.1	17
69	Experimental, theoretical and computational investigation of the inelastic neutron scattering spectrum of a homonuclear diatomic molecule in a nearly spherical trap: $\text{H}_2@C_{60}$. <i>Physical Chemistry Chemical Physics</i> , 2016, 18, 29369-29380.	1.3	17
70	Solid wetting-layers in inorganic nano-reactors: the water in imogolite nanotube case. <i>Nanoscale Advances</i> , 2020, 2, 1869-1877.	2.2	17
71	Lattice dynamics of a rotor-stator molecular crystal: Fullerene-cubane C_{60} . <i>Physical Review B</i> , 2010, 82, .	1.1	16
72	Hydrogen storage mechanism and lithium dynamics in $\text{Li}_{12}\text{C}_{60}$ investigated by ^1H SR. <i>Carbon</i> , 2015, 90, 130-137.	5.4	16

#	ARTICLE	IF	CITATIONS
73	Hydrogen motions in defective graphene: the role of surface defects. Physical Chemistry Chemical Physics, 2016, 18, 24820-24824.	1.3	16
74	Tunable intertube spacing in single-walled carbon nanotube bundles. Physical Review B, 2005, 72, .	1.1	15
75	Inelastic neutron scattering due to acoustic vibrations confined in nanoparticles: Theory and experiment. Physical Review B, 2008, 78, .	1.1	15
76	Understanding of ultra-cold neutron production in solid deuterium. Europhysics Letters, 2010, 92, 62001.	0.7	15
77	Lithium diffusion in $L_{i_2}X$		

#	ARTICLE	IF	CITATIONS
91	Spin-phonon coupling and high-temperature phase transition in multiferroic material YMnO_3 . Journal of Materials Chemistry C, 2015, 3, 11717-11728.	2.7	12
92	Lattice dynamics of pressure-polymerized phases of C60 : A neutron scattering investigation. Physical Review B, 2004, 70, .	1.1	11
93	Hydrogen in N-Methylacetamide: Positions and Dynamics of the Hydrogen Atoms Using Neutron Scattering. Journal of Physical Chemistry B, 2007, 111, 7725-7734.	1.2	11
94	Tetrahedron dynamics in the icosahedral quasicrystals $i\text{-ZnMgSc}$ and $i\text{-ZnAgSc}$ and the cubic $1/1$ -approximant Zn_6Sc . Journal of Physics Condensed Matter, 2013, 25, 115405.	0.7	11
95	The Endofullerene HF@C60 : Inelastic Neutron Scattering Spectra from Quantum Simulations and Experiment, Validity of the Selection Rule, and Symmetry Breaking. Journal of Physical Chemistry Letters, 2019, 10, 5365-5371.	2.1	11
96	Phonons and lithium diffusion in LiAlO_2 . Physical Review B, 2021, 103, .		
97	Diffraction of oriented nano-peapods. European Physical Journal B, 2006, 49, 147-155.	0.6	10
98	Unravelling low lying phonons and vibrations of carbon nanostructures: The contribution of inelastic and quasi-elastic neutron scattering. European Physical Journal: Special Topics, 2012, 213, 77-102.	1.2	10
99	Soft-phonon dynamics of the thermoelectric $\text{Pb}_2\text{-SnSe}$ at high temperatures. Physics Letters, Section A: General, Atomic and Solid State Physics, 2018, 382, 1937-1941.	0.9	10
100	Lattice Dynamics of Oligo(phenylenethienylene)s: A Far-Infrared and Inelastic Neutron Scattering Study. Journal of Physical Chemistry B, 2009, 113, 4197-4202.	1.2	9
101	Structure and dynamics of the fullerene polymer Li_4C_{60} studied with neutron scattering. Physical Review B, 2015, 92, .	1.1	9
102	Investigating anomalous thermal expansion of copper halides by inelastic neutron scattering and ab initio phonon calculations. Physical Chemistry Chemical Physics, 2017, 19, 12107-12116.	1.3	9
103	The structure, methyl rotation reflected in inelastic and quasielastic neutron scattering and vibrational spectra of 1,2,3,5-tetramethoxybenzene and its 2:1 complex with 1,2,4,5-tetracyanobenzene. Unconventional behavior of the C_6D_6 . C_6D_6 C_6D_6	1.2	8
104	Progressive melting in confined one-dimensional Pt_3C_{60} chains. Physical Review B, 2012, 86, .	1.1	8
105	Central Atom Size Effects on the Methyl Torsions of Group XIV Tetratoxides. Chemistry - A European Journal, 2012, 18, 13018-13024.	1.7	8
107	Inelastic neutron scattering an ab-initio calculation of negative thermal expansion in Ag_2O . Physica B: Condensed Matter, 2012, 407, 2146-2149.	1.3	8
108	Dynamics of the phase-change material GeTe across the structural phase transition. Frontiers of Physics, 2019, 14, 1.	2.4	8

#	ARTICLE	IF	CITATIONS
109	Lattice dynamics of the icosahedral quasicrystals i-ZnMgSc and i-ZnAgSc and the cubic 1/1-approximant Zn ₆ Sc. Journal of Physics Condensed Matter, 2014, 26, 055402.	0.7	7
110	Solidlike to liquidlike behavior of Cu diffusion in superionic X_{2Cu} . X_{2Cu} . Journal of Physics Condensed Matter, 2014, 26, 055402.	0.9	7
111	Melting mechanism of monolayers adsorbed in cylindrical pores: The influence of the pore wall roughness. Journal of Chemical Physics, 2008, 128, 184703.	1.2	6
112	Study of C ₆₀ Peapods After a High-Pressure "High-Temperature Treatment. Fullerenes Nanotubes and Carbon Nanostructures, 2010, 18, 412-416.	1.0	6
113	Neutron scattering and ^{13}C NMR investigations of the low temperature state of LuCuGaO ₄ . Journal of Physics Condensed Matter, 2013, 25, 356002.	0.7	6
114	Manipulation of the crystalline phase diagram of hydrogen through nanoscale confinement effects in porous carbons. Nanoscale, 2022, 14, 7250-7261.	2.8	6
115	The structure of diaminodurene and the dynamics of the methyl groups. Journal of Chemical Physics, 2009, 130, 164519.	1.2	5
116	Nanometric confinement: Toward new physical properties and technological developments. European Physical Journal: Special Topics, 2012, 213, 129-148.	1.2	5
117	From a one-dimensional crystal to a one-dimensional liquid: A comprehensive dynamical study of C ₆₀ peapods. Physical Review B, 2013, 87, .	1.1	5
118	Vibrational properties and phonon anharmonicity in ZnS _{1-x} Sex: Inelastic neutron scattering, Raman scattering, X-ray diffraction measurements and lattice dynamical studies. Physica B: Condensed Matter, 2014, 433, 149-156.	1.3	5
119	Neutron scattering study of nickel decorated thermally exfoliated graphite oxide. International Journal of Hydrogen Energy, 2019, 44, 30999-31007.	3.8	5
120	Structure and dynamics of single-wall-carbon nanotubes probed by neutron scattering. Physica B: Condensed Matter, 2000, 276-278, 276-277.	1.3	4
121	Melting mechanism of monolayers adsorbed in cylindrical pores: An influence of the pore wall roughness. Applied Surface Science, 2007, 253, 5601-5605.	3.1	4
122	High Pressure Phase Transitions in Yttria, Y ₂ O ₃ . Journal of Physics: Conference Series, 2012, 377, 012036.	0.3	4
123	Phonon "magnon coupling in CoF ₂ investigated by time-of-flight neutron spectroscopy. Solid State Communications, 2013, 174, 55-62.	0.9	4
124	First neutron studies of the magnetism and rattling modes in CePt ₄ Ge ₁₂ . Journal of Physics: Conference Series, 2015, 592, 012011.	0.3	4
125	Introduction of fractal absorbing boundary conditions in electromagnetic simulation by SMM. Modelling and Simulation in Materials Science and Engineering, 1998, 6, 111-121.	0.8	3
126	Effect of Nd and Rh substitution on the spin dynamics of the Kondo-insulator CeFe ₂ Al ₁₀ . Physical Review B, 2020, 102, .	1.1	3

#	ARTICLE	IF	CITATIONS
127	Spinâ€phonon coupling and thermodynamic behaviour in YCrO ₃ and LaCrO ₃ : inelastic neutron scattering and lattice dynamics. Journal of Physics Condensed Matter, 2020, 32, 505402.	0.7	3
128	Dynamical disorder and reorientation of the CH ₃ groups in N-methylacetamide. Physica B: Condensed Matter, 2004, 350, E587-E589.	1.3	2
129	Lowâ€Frequency Phonons in Highâ€Pressure Highâ€Temperature C ₆₀ Polymers. Fullerenes Nanotubes and Carbon Nanostructures, 2005, 12, 263-268.	1.0	2
130	Spectroscopies on Carbon Nanotubes. , 2006, , 277-334.		2
131	Crystal field manifestation in inelastic neutron scattering, magnetic susceptibility and specific heat of the antiferromagnetic CeCoAl ₄ . Journal of Magnetism and Magnetic Materials, 2013, 345, 243-248.	1.0	2
132	In situ X-ray diffraction observation of two-step fullerene coalescence in carbon peapods. Europhysics Letters, 2013, 103, 66002.	0.7	2
133	Phonons and oxygen diffusion in Bi ₂ O ₃ and (Bi _{0.7} Y _{0.3}) ₂ O ₃ . Journal of Physics Condensed Matter, 2020, 32, 334002.	0.7	2
134	Structure and vibrational properties of single wall carbon nanotubes. Synthetic Metals, 1999, 103, 2537-2539.	2.1	1
135	On the Raman Spectrum of Nanobundles of Single Wall Carbon Nanotubes. Materials Research Society Symposia Proceedings, 1999, 593, 107.	0.1	1
136	Probing the Dynamics of C ₆₀ Encaged Inside Singleâ€Walled Carbon Nanotubes by Inelastic Neutron Scattering. Fullerenes Nanotubes and Carbon Nanostructures, 2008, 16, 463-470.	1.0	1
137	Search for Light-Induced Intrinsic Localized Modes: Negative Result. Ferroelectrics, 2012, 440, 42-46.	0.3	1
138	Analysis of the magnetic properties of Ce ₃ Pt ₂₃ Si ₁₁ : orthorhombic crystal field and mean-field approximation. Journal of Physics Condensed Matter, 2018, 30, 285802.	0.7	1
139	From Heavy Fermion and Spin-Glass Behavior to Magnetic Order in CeT ₄ M Compounds. Acta Physica Polonica A, 2012, 121, 1014-1018.	0.2	1
140	Molecular dynamics of single wall nanotubes. , 1998, , .		0
141	Structure of singlewall carbon nanotubes: neutron powder diffraction and simulations.. Synthetic Metals, 1999, 103, 2517-2518.	2.1	0
142	The Vibrational Density-of-States of Nanobundles of Single Wall Carbon Nanotubes: An Inelastic Neutron Scattering Study. Materials Research Society Symposia Proceedings, 1999, 593, 101.	0.1	0
143	Neutron scattering studies of carbon nanotubes. , 1999, , .		0
144	Structure and dynamics of carbon buckyballs encapsulated into Single-Walled carbon Nanotubes. Materials Research Society Symposia Proceedings, 2004, 858, 22.	0.1	0

#	ARTICLE	IF	CITATIONS
145	Neutron diffraction study of p-phenylene oligomer molecules adsorbed onto graphite. Thin Solid Films, 2010, 518, 3786-3791.	0.8	0
146	Inelastic Neutron Scattering and Ab-Initio Calculation of Negative Thermal Expansion in Ag ₂ O., 2011, , .		0
147	Translational Dynamics of One-Dimensional Fullerene Chains Encapsulated Inside Single-Walled Carbon Nanotubes. Fullerenes Nanotubes and Carbon Nanostructures, 2012, 20, 395-400.	1.0	0
148	Atomic Dynamics in Complex Metallic Alloys. Materials Research Society Symposia Proceedings, 2013, 1517, 1.	0.1	0
149	Phonons et vibrations dans les fullérènes, les nanotubes de carbone et leurs composés., 2010, , .		0
150	Dynamical Flexibility in the Periodic Zn ₆ Sc _{1/1} -Approximant., 2013, , 253-259.		0