Elena F Sheka

List of Publications by Year
in descending order

147 papers	1,889 citations	279487 23 h-index	377514 34 g-index
148 all docs	148 docs citations	148 times ranked	1032 citing authors

#	Article	IF	Citations
1	Phonon dispersion in d8-naphthalene crystal at 6K. Journal of Physics C: Solid State Physics, 1980, 13, 4265-4283.	1.5	88
2	Spectroscopy of Molecular Excitons. Springer Series in Chemical Physics, 1985, , .	0.2	81
3	The 12 external and the 4 lowest internal phonon dispersion branches in d10-anthracene at 12K. Journal of Physics C: Solid State Physics, 1982, 15, 2353-2365.	1.5	55
4	Structure of Exciton Bands in Crystalline Anthracene. Physica Status Solidi (B): Basic Research, 1965, 11, 877-890.	0.7	50
5	Graphene Domain Signature of Raman Spectra of sp2 Amorphous Carbons. Nanomaterials, 2020, 10, 2021.	1.9	50
6	Shungite as the natural pantry of nanoscale reduced graphene oxide. International Journal of Smart and Nano Materials, 2014, 5, 1-16.	2.0	47
7	A New Approach to the Vibronic Spectra of Molecular Crystals. Physica Status Solidi (B): Basic Research, 1967, 19, 395-406.	0.7	37
8	Pressure dependence of phonon energies in d8-naphthalene. Journal of Physics C: Solid State Physics, 1981, 14, 1025-1041.	1.5	35
9	Broken symmetry approach and chemical susceptibility of carbon nanotubes. International Journal of Quantum Chemistry, 2010, 110, 1466-1480.	1.0	33
10	ELECTRON-VIBRATIONAL SPECTRA OF MOLECULES AND CRYSTALS. Uspekhi Fizicheskikh Nauk, 1972, 14, 484-511.	0.3	32
11	Deformation of Poly(dimethylsiloxane) Oligomers under Uniaxial Tension:â€‰ Quantum Chemical View. Journal of Physical Chemistry A, 1999, 103, 11355-11365.	1.1	32
12	Determination of phonon eigenvectors in naphthalene by fitting neutron scattering intensities. Molecular Physics, 1980, 39, 251-260.	0.8	31
13	Chemical susceptibility of fullerenes in view of Hartreeâ€“Fock approach. International Journal of Quantum Chemistry, 2007, 107, 2803-2816.	1.0	31
14	Molecular theory of graphene oxide. Physical Chemistry Chemical Physics, 2013, 15, 13304.	1.3	31
15	Optical limiters and diffraction elements based on a COANP-fullerene system: Nonlinear optical properties and quantum-chemical simulation. Optics and Spectroscopy (English Translation of Optika I) Tj ETQq1 1 0.784314 rgBT /O		
16	Donorâ€“acceptor interaction and fullerene C60 dimerization. Chemical Physics Letters, 2007, 438, 119-126.	1.2	30
17	Inelastic incoherent neutron scattering spectra at different temperatures and computer experiment for external phonon modes of naphthalene crystals. Physica Status Solidi (B): Basic Research, 1978, 85, 331-342.	0.7	29
18	sp amorphous carbons in view of multianalytical consideration: Normal, expeÑted and new. Journal of Non-Crystalline Solids, 2019, 524, 119608.	1.5	29

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19	Continuous Symmetry of C₆₀ Fullerene and Its Derivatives. Journal of Physical Chemistry A, 2011, 115, 3480-3490.	1.1	27
20	Dispersion of low frequency phonons in the deuterated naphthalene crystal. Solid State Communications, 1977, 23, 89-93.	0.9	25
21	Odd electrons and covalent bonding in fullerenes. International Journal of Quantum Chemistry, 2004, 100, 375-387.	1.0	25
22	Fractals of graphene quantum dots in photoluminescence of shungite. Journal of Experimental and Theoretical Physics, 2014, 118, 735-746.	0.2	24
23	NANOPACK: Parallel codes for semiempirical quantum chemical calculations of large systems in thesp-andspd-basis. International Journal of Quantum Chemistry, 2002, 88, 449-462.	1.0	23
24	Broken spin symmetry approach to chemical reactivity and magnetism of graphenium species. Journal of Experimental and Theoretical Physics, 2010, 110, 121-132.	0.2	23
25	Graphene-Carbon Nanotube Composites. Journal of Computational and Theoretical Nanoscience, 2010, 7, 1814-1824.	0.4	23
26	Technical graphene (reduced graphene oxide) and its natural analog (shungite). Technical Physics, 2016, 61, 1032-1038.	0.2	23
27	Anharmonicity of phonons in crystalline naphthalene. Journal of Physics C: Solid State Physics, 1984, 17, 5893-5914.	1.5	22
28	Intermolecular interaction in C60-based electron donor-acceptor complexes. International Journal of Quantum Chemistry, 2004, 100, 388-406.	1.0	22
29	Why sp²â€like nanosilicons should not form: Insight from quantum chemistry. International Journal of Quantum Chemistry, 2013, 113, 612-618.	1.0	22
30	Neutron Spectroscopy of Naphthalene Crystal Internal Phonon Modes. Physica Status Solidi (B): Basic Research, 1976, 75, 105-116.	0.7	21
31	â€œChemical portraitâ€•of fullerene molecules. Journal of Structural Chemistry, 2006, 47, 593-599.	0.3	21
32	The uniqueness of physical and chemical natures of graphene: Their coherence and conflicts. International Journal of Quantum Chemistry, 2014, 114, 1079-1095.	1.0	21
33	Viberational spectroscopy of dispersed silica: inelastic neutron scattering. Journal of Electron Spectroscopy and Related Phenomena, 1990, 54-55, 855-876.	0.8	20
34	High-spin silicon fullerene Si60 and its oligomers. International Journal of Quantum Chemistry, 2002, 88, 441-448.	1.0	20
35	Bond Length Effect on Odd-Electron Behavior in Single-Walled Carbon Nanotubes. Journal of Physical Chemistry C, 2007, 111, 10771-10779.	1.5	20
36	Inelastic incoherent neutron scattering from crystalline benzene. Societa Italiana Di Fisica Nuovo Cimento B-General Physics, Relativity Astronomy and Mathematical Physics and Methods, 1978, 44, 324-336.	0.2	19

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37	Techonological polymorphism of disperse amorphous silicas: inelastic neutron scattering and computer modelling. Russian Chemical Reviews, 1995, 64, 389-414.	2.5	19
38	Odd-electron molecular theory of graphene hydrogenation. Journal of Molecular Modeling, 2012, 18, 3751-3768.	0.8	19
39	Eigenvectors of low frequency internal phonons in crystalline anthracene-d10. Chemical Physics, 1981, 57, 407-414.	0.9	18
40	Stepwise computational synthesis of fullerene C60 derivatives. Fluorinated fullerenes C60F2k. Journal of Experimental and Theoretical Physics, 2010, 111, 397-414.	0.2	18
41	C60-based composites in view of topochemical reactions. Journal of Materials Chemistry, 2011, 21, 17128.	6.7	18
42	Physics and chemistry of graphene. Emergentness, magnetism, mechanophysics and mechanochemistry. Physics-Uspekhi, 2018, 61, 645-691.	0.8	18
43	Computationally Supported Neutron Scattering Study of Parent and Chemically Reduced Graphene Oxide. Journal of Physical Chemistry C, 2015, 119, 18650-18662.	1.5	17
44	Stretching and Breaking of Chemical Bonds, Correlation of Electrons, and Radical Properties of Covalent Species. Advances in Quantum Chemistry, 2015, 70, 111-161.	0.4	16
45	Graphene-nanotube structures: Constitution and formation energy. JETP Letters, 2009, 89, 352-356.	0.4	15
46	Mechanochemical Reaction in Graphane under Uniaxial Tension. Journal of Physical Chemistry C, 2011, 115, 23745-23754.	1.5	15
47	Highspin molecular magnetism of silicon surfaces. Surface Science, 2003, 532-535, 754-758.	0.8	14
48	Computational synthesis of hydrogenated fullerenes from C60 to C60H60. Journal of Molecular Modeling, 2011, 17, 1973-1984.	0.8	14
49	Computational strategy for graphene: Insight from odd electrons correlation. International Journal of Quantum Chemistry, 2012, 112, 3076-3090.	1.0	14
50	Some phonon shifts and widths in d8-naphthalene. Journal of Physics C: Solid State Physics, 1982, 15, 6533-6544.	1.5	13
51	Evolution of the coherence of vibrational states in a gradual disorder-order phase transition. Journal of Molecular Structure, 1984, 114, 325-328.	1.8	13
52	ADSORPTION MODELING OF POLYDIMETHYLSILOXANE ON SILICA: SEMIEMPIRICAL QUANTUM-CHEMICAL CALCULATIONS. Surface Review and Letters, 1997, 04, 879-883.	0.5	13
53	Optical spectra and covalent chemistry of fulleropyrrolidines. International Journal of Quantum Chemistry, 2007, 107, 2787-2802.	1.0	13
54	A tricotage-like failure of nanographene. Journal of Molecular Modeling, 2011, 17, 1121-1131.	0.8	13

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55	Computationally Supported Neutron Scattering Study of Natural and Synthetic Amorphous Carbons. Journal of Physical Chemistry C, 2019, 123, 15841-15850.	1.5	13
56	Temperature dependence of the phonon frequencies in deuterated anthracene. Journal of Physics C: Solid State Physics, 1982, 15, 7283-7294.	1.5	12
57	From Molecules to Particles: Quantum-chemical View Applied to Fumed Silica. Journal of Nanoparticle Research, 1999, 1, 71-81.	0.8	12
58	Nanostructural magnetism of polymeric fullerene crystals. Journal of Experimental and Theoretical Physics, 2006, 103, 728-739.	0.2	12
59	Structure-sensitive mechanism of nanographene failure. Journal of Experimental and Theoretical Physics, 2011, 112, 602-611.	0.2	12
60	Intermolecular interactions of polydimethylsiloxane oligomers with hydroxylated and silylated fumed silica. Composite Interfaces, 1998, 6, 3-17.	1.3	11
61	Odd electrons in molecular chemistry, surface science, and solid state magnetism. International Journal of Quantum Chemistry, 2007, 107, 2935-2955.	1.0	11
62	Electronic structure and spectra of N-methylfullerenepyrrolidine. Optics and Spectroscopy (English) Tj ETQq0 0 0 rgBT /Overlock 10 Tf 5	0.2	11
63	Spectroscopy of amorphous substances with molecular structure. Uspekhi Fizicheskikh Nauk, 1990, 33, 147-166.	0.3	10
64	Neutron spectroscopy of water adsorbed on silica. Physica B: Condensed Matter, 1991, 174, 182-186.	1.3	10
65	Computational INS spectroscopy of dispersed catalysts. Physica B: Condensed Matter, 1991, 174, 227-232.	1.3	10
66	Isotopic effect in the absorption spectra of naphthalene crystal. Chemical Physics, 1975, 8, 99-111.	0.9	9
67	Fullerenes as polyradicals. Open Physics, 2004, 2, .	0.8	9
68	Fullerene-cluster amplifiers and nanophotonics of fullerene solutions. Journal of Nanophotonics, 2009, 3, 033501.	0.4	9
69	Neutron scattering study of reduced graphene oxide of natural origin. JETP Letters, 2014, 99, 650-655.	0.4	9
70	Vibronic Absorption with Totally Symmetrical Phonons in Naphthalene Crystal. Molecular Crystals and Liquid Crystals, 1978, 47, 119-143.	0.9	8
71	Adducts AnC60Hn: Electroâ€optical Properties and Quantum Chemical Calculation Data. Fullerenes Nanotubes and Carbon Nanostructures, 2006, 14, 343-348.	1.0	8
72	Donorâ€“acceptor origin of fullerene C60 dimerization. International Journal of Quantum Chemistry, 2007, 107, 2361-2371.	1.0	8

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73	Harmonic Dynamics of Anthracene Crystal. Molecular Crystals and Liquid Crystals, 1984, 104, 207-230.	0.9	7
74	INS study of itermolecular interaction at the silicone-fumed silica interface. Physica B: Condensed Matter, 2000, 276-278, 244-246.	1.3	7
75	sp2 Carbon Stable Radicals. Journal of Carbon Research, 2021, 7, 31.	1.4	7
76	Spin Chemical Physics of Graphene. , 0, , .		7
77	Neutron scattering from water adsorbed on ultrafine nickel particles. Physica B: Condensed Matter, 1991, 174, 187-191.	1.3	6
78	Water on amorphous silicas: INS study. Physica B: Condensed Matter, 1992, 180-181, 522-524.	1.3	6
79	Influence of spin-orbit interaction on magnetic properties of fullerenes. European Physical Journal D, 2016, 70, 1.	0.6	6
80	Graphene Oxyhydride Catalysts in View of Spin Radical Chemistry. Materials, 2020, 13, 565.	1.3	6
81	Amplitude weighted density of bulk and surface vibrations; ultrafine nickel particles. Journal of Electron Spectroscopy and Related Phenomena, 1990, 54-55, 425-443.	0.8	5
82	Surface vibrations of silicon nitride: Inelastic neutron scattering study and computer modeling. Journal of Electron Spectroscopy and Related Phenomena, 1994, 67, 133-139.	0.8	5
83	Fullerene model of silicon nanofibers. JETP Letters, 2001, 74, 177-181.	0.4	5
84	Photosynthetic reactions in fullerene based donor-acceptor complexes. Journal of Structural Chemistry, 2006, 47, 600-607.	0.3	5
85	Carboxylic species adsorption on TiO2 nanoparticles. Physics of the Solid State, 2007, 49, 154-163.	0.2	5
86	On the donor-acceptor interaction and electron transfer at the titanium oxide-organic dye interface. Physics of the Solid State, 2007, 49, 2004-2009.	0.2	5
87	Shpolski effect in optical spectra of frozen solutions of the organic C60 fullerene derivative in toluene. Physics of the Solid State, 2009, 51, 1315-1319.	0.2	5
88	Computational synthesis of C60 cyano- and azopolyderivatives. Journal of Molecular Modeling, 2012, 18, 1409-1420.	0.8	5
89	Topochemistry of Spatially Extended sp 2 Nanocarbons: Fullerenes, Nanotubes, and Graphene. Carbon Materials, 2013, , 137-197.	0.2	5
90	Virtual Vibrational Spectrometry of Stable Radicalsâ€"Necklaced Graphene Molecules. Nanomaterials, 2022, 12, 597.	1.9	5

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91	Exciton-phonon interaction and energy transfer in benzene and isotopically impure deuterobenzene crystals. Journal of Luminescence, 1974, 8, 349-358.	1.5	4
92	Pressure dependence of lattice frequencies of deuterated naphthalene at 100 K. Physica Status Solidi (B): Basic Research, 1979, 91, K27.	0.7	4
93	Ordered and disordered states of DOBHOP. Physica Status Solidi A, 1981, 63, 265-269.	1.7	4
94	Computer modeling of amorphous silica structures. Reaction Kinetics and Catalysis Letters, 1993, 50, 389-414.	0.6	4
95	Computational modeling of amorphous silica. 2. Modeling the initial structures. Aerosil. Journal of Structural Chemistry, 1994, 35, 291-298.	0.3	4
96	Density of vibrational states of silicon nitride. Physica B: Condensed Matter, 1994, 198, 200-202.	1.3	4
97	Computational investigation of the influence of the environment on mechanical properties of solids. International Journal of Quantum Chemistry, 1995, 56, 161-173.	1.0	4
98	Nanomaterials: Reality and computational modelling. Scripta Materialia, 1995, 6, 803-806.	0.5	4
99	Intermolecular Interaction and Vibrational Spectra at Fumed Silica Particles/Silicone Polymer Interface. Journal of Nanoparticle Research, 2003, 5, 419-437.	0.8	4
100	NANOVIBR: Parallel codes for semiempirical quantum chemical and harmonic vibration large-scale calculations. International Journal of Quantum Chemistry, 2004, 96, 73-79.	1.0	4
101	Chemical reactivity and magnetism of graphene. International Journal of Quantum Chemistry, 2010, 110, 1938-1946.	1.0	4
102	The nature of enhanced linear and nonlinear optical effects in fullerene solutions. Journal of Experimental and Theoretical Physics, 2009, 108, 738-750.	0.2	4
103	Virtual Vibrational Analytics of Reduced Graphene Oxide. International Journal of Molecular Sciences, 2022, 23, 6978.	1.8	4
104	Asymmetry of phonon side bands of optical transitions in impurity molecular crystals caused by a change in external phonon frequencies. Physica Status Solidi (B): Basic Research, 1976, 78, K1.	0.7	3
105	Excitonâ€"Phonon Luminescence of Perfect and Doped Naphthalene Crystals. Molecular Crystals and Liquid Crystals, 1980, 57, 65-87.	0.9	3
106	Neutron Scattering from Equilibrium and Non-equilibrium Phonons, Excitons and Polaritons. Molecular Crystals and Liquid Crystals, 1980, 57, 145-161.	0.9	3
107	Spectroscopy of Molecular Crystals: A Bibliography for 1981. Molecular Crystals and Liquid Crystals, 1984, 104, 1-94.	0.9	3
108	Computational modeling of amorphous silica. 3. Modeling the initial structures. Silica gel. Journal of Structural Chemistry, 1994, 35, 299-304.	0.3	3

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109	Density of vibrational states of thiol capped CdS particles. Inelastic neutron scattering. Physica B: Condensed Matter, 1994, 198, 197-199.	1.3	3
110	Computer modeling of assembly of atoms in an electric field. International Journal of Quantum Chemistry, 1996, 57, 741-755.	1.0	3
111	Quantum-chemical study of the interface formed by carboxylic species on TiO2 nanoparticles. 1. Nanoparticle surface. Journal of Nanoparticle Research, 2005, 7, 171-186.	0.8	3
112	Nanophotonics of Fullerene. 1. Chemistry and Medicine. Nanoscience and Nanotechnology Letters, 2011, 3, 28-33.	0.4	3
113	SIXTH ALL-UNION SEMINAR ON "EXCITONS IN CRYSTALS". Uspekhi Fizicheskikh Nauk, 1972, 14, 530-532.	0.3	2
114	Spectroscopy of Molecular Crystals: A Bibliography for 1971. Molecular Crystals and Liquid Crystals, 1973, 19, 331-367.	0.9	2
115	Multiphonon absorption in molecular crystals. Physica Status Solidi (B): Basic Research, 1976, 78, 325-333.	0.7	2
116	Comparative analysis of vibration spectra of dispersive silicas and their components. Journal of Structural Chemistry, 1994, 34, 523-533.	0.3	2
117	Computational chemistry of the silicon nitride surface. 1. Water, ammonia, and water-ammonia complex. Journal of Structural Chemistry, 1995, 36, 50-59.	0.3	2
118	Multi-mode ground state interaction terms in C60-based electron donor-acceptor complexes. Open Physics, 2004, 2, .	0.8	2
119	Fullerene nanoclusters as enhancers in linear spectroscopy and nonlinear optics. High Energy Chemistry, 2009, 43, 628-633.	0.2	2
120	Influence of the structure of fullerene molecules on their clusterization in the crystalline matrix. Physics of the Solid State, 2009, 51, 2193-2198.	0.2	2
121	Dirac Material Graphene. Reviews on Advanced Materials Science, 2018, 53, 1-28.	1.4	2
122	The electronic states of naphthalene molecules adsorbed on a zeolite. Theoretical and Experimental Chemistry, 1969, 3, 220-223.	0.2	1
123	Vibrational spectroscopy of dispersed silica: Aerosil. Journal of Structural Chemistry, 1993, 33, 536-544.	0.3	1
124	Vibrations of dispersed silicas: A comparative. Reaction Kinetics and Catalysis Letters, 1993, 50, 221-226.	0.6	1
125	Computational modeling of amorphous silica. 4. Modeling the initial structures. Aerogel. Journal of Structural Chemistry, 1994, 35, 305-308.	0.3	1
126	Computational modeling of amorphous silica. 1. Modeling the starting structures. A general conception. Journal of Structural Chemistry, 1994, 35, 215-223.	0.3	1

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127	Surface magnetism of silicon [111](7/spl times/7) and [001](2/spl times/1) surfaces: quantum-chemical approach. , 1999, , .		1
128	Fullerenes as polyradicals. Future Generation Computer Systems, 2004, 20, 749-762.	4.9	1
129	Fullerene-silica complexes for medical chemistry. Russian Journal of Physical Chemistry A, 2007, 81, 959-966.	0.1	1
130	Vibronic resonance in spectra of frozen solutions of the C60 fullerene derivatives. Physics of the Solid State, 2011, 53, 1307-1313.	0.2	1
131	Spin-orbit coupling of sp2 nanocarbons and magnetism of fullerene C60 in view of spin peculiarities of unrestricted Hartreeâ€“Fock solution. Fullerenes Nanotubes and Carbon Nanostructures, 2017, 25, 289-294.	1.0	1
132	Highâ€spin silicon fullerene Si60 and its oligomers. International Journal of Quantum Chemistry, 2002, 88, 441-448.	1.0	1
133	Computational Modeling of Surface Layers of Refractory Compounds. , 1999, , 155-186.		1
134	Nanophotonics of Fullerene. 2. Linear and Non-Linear Optics. Nanoscience and Nanotechnology Letters, 2011, 3, 34-40.	0.4	1
135	Luminescence spectra and adsorption characteristics of naphthalene on various metal-substituted forms of type X zeolite. Theoretical and Experimental Chemistry, 1972, 5, 156-158.	0.2	0
136	Vladimir L'vovich Broude (Obituary). Uspekhi Fizicheskikh Nauk, 1979, 22, 292-293.	0.3	0
137	Method for the construction of basis spectra of multicomponent systems. The zero correlation coefficient criterion. Journal of Structural Chemistry, 1993, 34, 37-45.	0.3	0
138	Construction of vibrational basis spectra of multicomponent systems 1. Aerosil. Journal of Structural Chemistry, 1993, 34, 46-55.	0.3	0
139	Construction of vibrational basis spectra of multicomponent systems 2. Silica gel. Journal of Structural Chemistry, 1993, 34, 56-67.	0.3	0
140	Construction of basis vibration spectra of multicomponent systems. 3. Aerogel. Journal of Structural Chemistry, 1994, 34, 513-522.	0.3	0
141	Computational chemistry of the silicon nitride surface. 2. Binary hydroxylamine complexes. Geometry and bond energies. Journal of Structural Chemistry, 1996, 37, 24-40.	0.3	0
142	Water at the interface modified silica filler-polydimethylsiloxane: quantum-chemical modelling. Composite Interfaces, 2001, 8, 291-306.	1.3	0
143	TUNCUR: Sequential codes for semiempirical quantum chemical calculations of tunneling current. International Journal of Quantum Chemistry, 2004, 100, 695-708.	1.0	0
144	Odd Electrons of Nanomaterials: A New Approach to Computational Chemical Engineering. AIP Conference Proceedings, 2007, , .	0.3	0

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145	10.1007/s11448-008-3004-2. , 2010, 87, 133.		0
146	DIRAC MATERIAL GRAPHENE. Radioelektronika, Nanosistemy, Informacionnye Tehnologii, 2016, 8, 131-153.	0.2	0
147	Spin Effects in sp 2 Nanocarbons in the Light of Unrestricted Hartree-Fock Approach and Spin-Orbit Coupling Theory. Progress in Theoretical Chemistry and Physics, 2017, , 39-63.	0.2	0