Elena F Sheka

List of Publications by Year in Descending Order

144 papers	1,593 citations	21 h-index	30 g-index
148 ext. papers	1,744 ext. citations	1.9 avg, IF	4.93 L-index

#	Paper	IF	Citations
144	Virtual Vibrational Spectrometry of Stable Radicals-Necklaced Graphene Molecules.. *Nanomaterials*, **2022**, 12,	5.4	1
143	sp2 Carbon Stable Radicals. *Journal of Carbon Research*, **2021**, 7, 31	3.3	4
142	Graphene Oxyhydride Catalysts in View of Spin Radical Chemistry. *Materials*, **2020**, 13,	3.5	3
141	Graphene Domain Signature of Raman Spectra of Amorphous Carbons. *Nanomaterials*, **2020**, 10,	5.4	15
140	sp amorphous carbons in view of multianalytical consideration: Normal, expe□ed and new. *Journal of Non-Crystalline Solids*, **2019**, 524, 119608	3.9	13
139	Computationally Supported Neutron Scattering Study of Natural and Synthetic Amorphous Carbons. *Journal of Physical Chemistry C*, **2019**, 123, 15841-15850	3.8	10
138	Dirac Material Graphene. *Reviews on Advanced Materials Science*, **2018**, 53, 1-28	4.8	1
137	Physics and chemistry of graphene. Emergentness, magnetism, mechanophysics and mechanochemistry. *Physics-Uspekhi*, **2018**, 61, 645-691	2.8	13
136	Spin-orbit coupling of sp2 nanocarbons and magnetism of fullerene C60 in view of spin peculiarities of unrestricted Hartree□ock solution. *Fullerenes Nanotubes and Carbon Nanostructures*, **2017**, 25, 289-294	1.8	1
135	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	0.6	
134	Influence of spin-orbit interaction on magnetic properties of fullerenes. *European Physical Journal D*, **2016**, 70, 1	1.3	2
133	Technical graphene (reduced graphene oxide) and its natural analog (shungite). *Technical Physics*, **2016**, 61, 1032-1038	0.5	17
132	Computationally Supported Neutron Scattering Study of Parent and Chemically Reduced Graphene Oxide. *Journal of Physical Chemistry C*, **2015**, 119, 18650-18662	3.8	14
131	Stretching and Breaking of Chemical Bonds, Correlation of Electrons, and Radical Properties of Covalent Species. *Advances in Quantum Chemistry*, **2015**, 70, 111-161	1.4	10
130	The uniqueness of physical and chemical natures of graphene: Their coherence and conflicts. *International Journal of Quantum Chemistry*, **2014**, 114, 1079-1095	2.1	20
129	Neutron scattering study of reduced graphene oxide of natural origin. *JETP Letters*, **2014**, 99, 650-655	1.2	8
128	Fractals of graphene quantum dots in photoluminescence of shungite. *Journal of Experimental and Theoretical Physics*, **2014**, 118, 735-746	1	19

127	Shungite as the natural pantry of nanoscale reduced graphene oxide. *International Journal of Smart and Nano Materials*, **2014**, 5, 1-16	3.6	33
126	Why sp2-like nanosilicons should not form: Insight from quantum chemistry. *International Journal of Quantum Chemistry*, **2013**, 113, 612-618	2.1	19
125	Molecular theory of graphene oxide. *Physical Chemistry Chemical Physics*, **2013**, 15, 13304-22	3.6	27
124	Topochemistry of Spatially Extended sp2 Nanocarbons: Fullerenes, Nanotubes, and Graphene. *Carbon Materials*, **2013**, 137-197		4
123	Odd-electron molecular theory of graphene hydrogenation. *Journal of Molecular Modeling*, **2012**, 18, 3751-68	2	19
122	Computational strategy for graphene: Insight from odd electrons correlation. *International Journal of Quantum Chemistry*, **2012**, 112, 3076-3090	2.1	14
121	Computational synthesis of C□□yano- and azopolyderivatives. *Journal of Molecular Modeling*, **2012**, 18, 1409-20	2	5
120	Mechanochemical Reaction in Graphane under Uniaxial Tension. *Journal of Physical Chemistry C*, **2011**, 115, 23745-23754	3.8	13
119	Continuous symmetry of C60 fullerene and its derivatives. *Journal of Physical Chemistry A*, **2011**, 115, 3480-90	2.8	20
118	C60-based composites in view of topochemical reactions. *Journal of Materials Chemistry*, **2011**, 21, 17128		16
117	Structure-sensitive mechanism of nanographene failure. *Journal of Experimental and Theoretical Physics*, **2011**, 112, 602-611	1	11
116	Vibronic resonance in spectra of frozen solutions of the C60 fullerene derivatives. *Physics of the Solid State*, **2011**, 53, 1307-1313	0.8	0
115	A tricotage-like failure of nanographene. *Journal of Molecular Modeling*, **2011**, 17, 1121-31	2	12
114	Computational synthesis of hydrogenated fullerenes from C□□o C□□□*Journal of Molecular Modeling*, **2011**, 17, 1973-84	2	12
113	Nanophotonics of Fullerene. 1. Chemistry and Medicine. *Nanoscience and Nanotechnology Letters*, **2011**, 3, 28-33	0.8	3
112	Broken spin symmetry approach to chemical reactivity and magnetism of graphenium species. *Journal of Experimental and Theoretical Physics*, **2010**, 110, 121-132	1	20
111	Stepwise computational synthesis of fullerene C60 derivatives. Fluorinated fullerenes C60F2k. *Journal of Experimental and Theoretical Physics*, **2010**, 111, 397-414	1	14
110	Graphene-Carbon Nanotube Composites. *Journal of Computational and Theoretical Nanoscience*, **2010**, 7, 1814-1824	0.3	16

109	Broken symmetry approach and chemical susceptibility of carbon nanotubes. *International Journal of Quantum Chemistry*, **2010**, 110, 1466-1480	2.1	30
108	Enhanced Raman scattering provided by fullerene nanoclusters **2010**, 87, 133		
107	Fullerene-cluster amplifiers and nanophotonics of fullerene solutions. *Journal of Nanophotonics*, **2009**, 3, 033501	1.1	7
106	Chemical reactivity and magnetism of graphene. *International Journal of Quantum Chemistry*, **2009**, 110, NA-NA	2.1	3
105	Fullerene nanoclusters as enhancers in linear spectroscopy and nonlinear optics. *High Energy Chemistry*, **2009**, 43, 628-633	0.9	1
104	Graphene-nanotube structures: Constitution and formation energy. *JETP Letters*, **2009**, 89, 352-356	1.2	12
103	The nature of enhanced linear and nonlinear optical effects in fullerene solutions. *Journal of Experimental and Theoretical Physics*, **2009**, 108, 738-750	1	2
102	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	0.8	4
101	Influence of the structure of fullerene molecules on their clusterization in the crystalline matrix. *Physics of the Solid State*, **2009**, 51, 2193-2198	0.8	1
100	Bond Length Effect on Odd-Electron Behavior in Single-Walled Carbon Nanotubes. *Journal of Physical Chemistry C*, **2007**, 111, 10771-10779	3.8	18
99	Donor□cceptor interaction and fullerene C60 dimerization. *Chemical Physics Letters*, **2007**, 438, 119-126	2.5	28
98	Chemical susceptibility of fullerenes in view of Hartree□ock approach. *International Journal of Quantum Chemistry*, **2007**, 107, 2803-2816	2.1	27
97	Optical spectra and covalent chemistry of fulleropyrrolidines. *International Journal of Quantum Chemistry*, **2007**, 107, 2787-2802	2.1	11
96	Donor□cceptor origin of fullerene C60 dimerization. *International Journal of Quantum Chemistry*, **2007**, 107, 2361-2371	2.1	5
95	Odd electrons in molecular chemistry, surface science, and solid state magnetism. *International Journal of Quantum Chemistry*, **2007**, 107, 2935-2955	2.1	10
94	Electronic structure and spectra of N-methylfullerenepyrrolidine. *Optics and Spectroscopy (English Translation of Optika I Spektroskopiya)*, **2007**, 102, 432-441	0.7	10
93	Fullerene-silica complexes for medical chemistry. *Russian Journal of Physical Chemistry A*, **2007**, 81, 959-966	0.7	1
92	Carboxylic species adsorption on TiO2 nanoparticles. *Physics of the Solid State*, **2007**, 49, 154-163	0.8	4

91	On the donor-acceptor interaction and electron transfer at the titanium oxide-organic dye interface. *Physics of the Solid State*, **2007**, 49, 2004-2009	0.8	5
90	Adducts AnC60Hn: Electro-optical Properties and Quantum Chemical Calculation Data. *Fullerenes Nanotubes and Carbon Nanostructures*, **2006**, 14, 343-348	1.8	7
89	Nanostructural magnetism of polymeric fullerene crystals. *Journal of Experimental and Theoretical Physics*, **2006**, 103, 728-739	1	8
88	Chemical portrait of fullerene molecules. *Journal of Structural Chemistry*, **2006**, 47, 593-599	0.9	18
87	Photosynthetic reactions in fullerene based donor-acceptor complexes. *Journal of Structural Chemistry*, **2006**, 47, 600-607	0.9	4
86	Quantum-chemical study of the interface formed by carboxylic species on TiO2 nanoparticles. 1. Nanoparticle surface. *Journal of Nanoparticle Research*, **2005**, 7, 171-186	2.3	3
85	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 Spektroskopiya)*, **2004**, 96, 599-612	0.7	24
84	Multi-mode ground state interaction terms in C60-based electron donor-acceptor complexes. *Open Physics*, **2004**, 2,	1.3	2
83	Fullerenes as polyradicals. *Open Physics*, **2004**, 2,	1.3	8
82	NANOVIBR: Parallel codes for semiempirical quantum chemical and harmonic vibration large-scale calculations. *International Journal of Quantum Chemistry*, **2004**, 96, 73-79	2.1	3
81	Odd electrons and covalent bonding in fullerenes. *International Journal of Quantum Chemistry*, **2004**, 100, 375-387	2.1	23
80	Intermolecular interaction in C60-based electron donor acceptor complexes. *International Journal of Quantum Chemistry*, **2004**, 100, 388-406	2.1	21
79	TUNCUR: Sequential codes for semiempirical quantum chemical calculations of tunneling current. *International Journal of Quantum Chemistry*, **2004**, 100, 695-708	2.1	
78	Fullerenes as polyradicals. *Future Generation Computer Systems*, **2004**, 20, 749-762	7.5	1
77	Intermolecular Interaction and Vibrational Spectra at Fumed Silica Particles/Silicone Polymer Interface. *Journal of Nanoparticle Research*, **2003**, 5, 419-437	2.3	3
76	Highspin molecular magnetism of silicon surfaces. *Surface Science*, **2003**, 532-535, 754-758	1.8	14
75	High-spin silicon fullerene Si60 and its oligomers. *International Journal of Quantum Chemistry*, **2002**, 88, 441-448	2.1	20
74	NANOPACK: Parallel codes for semiempirical quantum chemical calculations of large systems in the sp- and spd-basis. *International Journal of Quantum Chemistry*, **2002**, 88, 449-462	2.1	18

73	High-spin silicon fullerene Si60 and its oligomers **2002**, 88, 441		1
72	Fullerene model of silicon nanofibers. *JETP Letters*, **2001**, 74, 177-181	1.2	5
71	Water at the interface modified silica filler-polydimethylsiloxane: quantum-chemical modelling. *Composite Interfaces*, **2001**, 8, 291-306	2.3	
70	INS study of itermolecular interaction at the silicone-fumed silica interface. *Physica B: Condensed Matter*, **2000**, 276-278, 244-246	2.8	7
69	From Molecules to Particles: Quantum-chemical View Applied to Fumed Silica. *Journal of Nanoparticle Research*, **1999**, 1, 71-81	2.3	8
68	Surface magnetism of silicon [111](7/spl times/7) and [001](2/spl times/1) surfaces: quantum-chemical approach **1999**,		1
67	Deformation of Poly(dimethylsiloxane) Oligomers under Uniaxial Tension: Quantum Chemical View. *Journal of Physical Chemistry A*, **1999**, 103, 11355-11365	2.8	29
66	Computational Modeling of Surface Layers of Refractory Compounds **1999**, 155-186		1
65	Intermolecular interactions of polydimethylsiloxane oligomers with hydroxylated and silylated fumed silica. *Composite Interfaces*, **1998**, 6, 3-17	2.3	9
64	ADSORPTION MODELING OF POLYDIMETHYLSILOXANE ON SILICA: SEMIEMPIRICAL QUANTUM-CHEMICAL CALCULATIONS. *Surface Review and Letters*, **1997**, 04, 879-883	1.1	6
63	Computational chemistry of the silicon nitride surface. 2. Binary hydroxylamine complexes. Geometry and bond energies. *Journal of Structural Chemistry*, **1996**, 37, 24-40	0.9	
62	Computer modeling of assembly of atoms in an electric field. *International Journal of Quantum Chemistry*, **1996**, 57, 741-755	2.1	3
61	Computational chemistry of the silicon nitride surface. 1. Water, ammonia, and water-ammonia complex. *Journal of Structural Chemistry*, **1995**, 36, 50-59	0.9	1
60	Computational investigation of the influence of the environment on mechanical properties of solids. *International Journal of Quantum Chemistry*, **1995**, 56, 161-173	2.1	4
59	Techonological polymorphism of disperse amorphous silicas: inelastic neutron scattering and computer modelling. *Russian Chemical Reviews*, **1995**, 64, 389-414	6.8	16
58	Nanomaterials: Reality and computational modelling. *Scripta Materialia*, **1995**, 6, 803-806		4
57	Computational modeling of amorphous silica. 2. Modeling the initial structures. Aerosil. *Journal of Structural Chemistry*, **1994**, 35, 291-298	0.9	2
56	Computational modeling of amorphous silica. 3. Modeling the initial structures. Silica gel. *Journal of Structural Chemistry*, **1994**, 35, 299-304	0.9	3

55	Computational modeling of amorphous silica. 4. Modeling the initial structures. Aerogel. *Journal of Structural Chemistry*, **1994**, 35, 305-308	0.9	0
54	Computational modeling of amorphous silica. 1. Modeling the starting structures. A general conception. *Journal of Structural Chemistry*, **1994**, 35, 215-223	0.9	1
53	Construction of basis vibration spectra of multicomponent systems. 3. Aerogel. *Journal of Structural Chemistry*, **1994**, 34, 513-522	0.9	
52	Comparative analysis of vibration spectra of dispersive silicas and their components. *Journal of Structural Chemistry*, **1994**, 34, 523-533	0.9	2
51	Density of vibrational states of thiol capped CdS particles. Inelastic neutron scattering. *Physica B: Condensed Matter*, **1994**, 198, 197-199	2.8	3
50	Density of vibrational states of silicon nitride. *Physica B: Condensed Matter*, **1994**, 198, 200-202	2.8	3
49	Surface vibrations of silicon nitride: Inelastic neutron scattering study and computer modeling. *Journal of Electron Spectroscopy and Related Phenomena*, **1994**, 67, 133-139	1.7	5
48	Method for the construction of basis spectra of multicomponent systems. The zero correlation coefficient criterion. *Journal of Structural Chemistry*, **1993**, 34, 37-45	0.9	
47	Construction of vibrational basis spectra of multicomponent systems 1. Aerosil. *Journal of Structural Chemistry*, **1993**, 34, 46-55	0.9	
46	Construction of vibrational basis spectra of multicomponent systems 2. Silica gel. *Journal of Structural Chemistry*, **1993**, 34, 56-67	0.9	
45	Vibrational spectroscopy of dispersed silica: Aerosil. *Journal of Structural Chemistry*, **1993**, 33, 536-544	0.9	1
44	Vibrations of dispersed silicas: A comparative. *Reaction Kinetics and Catalysis Letters*, **1993**, 50, 221-226		1
43	Computer modeling of amorphous silica structures. *Reaction Kinetics and Catalysis Letters*, **1993**, 50, 389-414		3
42	Water on amorphous silicas: INS study. *Physica B: Condensed Matter*, **1992**, 180-181, 522-524	2.8	6
41	Neutron spectroscopy of water adsorbed on silica. *Physica B: Condensed Matter*, **1991**, 174, 182-186	2.8	10
40	Neutron scattering from water adsorbed on ultrafine nickel particles. *Physica B: Condensed Matter*, **1991**, 174, 187-191	2.8	6
39	Computational INS spectroscopy of dispersed catalysts. *Physica B: Condensed Matter*, **1991**, 174, 227-232	2.8	10
38	Amplitude weighted density of bulk and surface vibrations; ultrafine nickel particles. *Journal of Electron Spectroscopy and Related Phenomena*, **1990**, 54-55, 425-443	1.7	5

37	Viberational spectroscopy of dispersed silica: inelastic neutron scattering. *Journal of Electron Spectroscopy and Related Phenomena*, **1990**, 54-55, 855-876	1.7	20
36	Spectroscopy of amorphous substances with molecular structure. *Uspekhi Fizicheskikh Nauk*, **1990**, 33, 147-166		7
35	Spectroscopy of Molecular Excitons. *Springer Series in Chemical Physics*, **1985**,	0.3	66
34	Harmonic Dynamics of Anthracene Crystal. *Molecular Crystals and Liquid Crystals*, **1984**, 104, 207-230		4
33	Spectroscopy of Molecular Crystals: A Bibliography for 1981. *Molecular Crystals and Liquid Crystals*, **1984**, 104, 1-94		2
32	Anharmonicity of phonons in crystalline naphthalene. *Journal of Physics C: Solid State Physics*, **1984**, 17, 5893-5914		20
31	Evolution of the coherence of vibrational states in a gradual disorder-order phase transition. *Journal of Molecular Structure*, **1984**, 114, 325-328	3.4	12
30	Some phonon shifts and widths in d8-naphthalene. *Journal of Physics C: Solid State Physics*, **1982**, 15, 6533-6544		13
29	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		53
28	Temperature dependence of the phonon frequencies in deuterated anthracene. *Journal of Physics C: Solid State Physics*, **1982**, 15, 7283-7294		12
27	Pressure dependence of phonon energies in d8-naphthalene. *Journal of Physics C: Solid State Physics*, **1981**, 14, 1025-1041		34
26	Ordered and disordered states of DOBHOP. *Physica Status Solidi A*, **1981**, 63, 265-269		4
25	Eigenvectors of low frequency internal phonons in crystalline anthracene-d10. *Chemical Physics*, **1981**, 57, 407-414	2.3	16
24	Determination of phonon eigenvectors in naphthalene by fitting neutron scattering intensities. *Molecular Physics*, **1980**, 39, 251-260	1.7	29
23	Exciton–Phonon Luminescence of Perfect and Doped Naphthalene Crystals. *Molecular Crystals and Liquid Crystals*, **1980**, 57, 65-87		3
22	Neutron Scattering from Equilibrium and Non-equilibrium Phonons, Excitons and Polaritons. *Molecular Crystals and Liquid Crystals*, **1980**, 57, 145-161		0
21	Phonon dispersion in d8-naphthalene crystal at 6K. *Journal of Physics C: Solid State Physics*, **1980**, 13, 4265-4283		81
20	Pressure dependence of lattice frequencies of deuterated naphthalene at 100 K. *Physica Status Solidi (B): Basic Research*, **1979**, 91, K27-K29	1.3	4

19	Vladimir L'vovich Broude (Obituary). *Uspekhi Fizicheskikh Nauk*, **1979**, 22, 292-293		
18	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	1.3	27
17	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		19
16	Vibronic Absorption with Totally Symmetrical Phonons in Naphthalene Crystal. *Molecular Crystals and Liquid Crystals*, **1978**, 47, 119-143		8
15	Dispersion of low frequency phonons in the deuterated naphthalene crystal. *Solid State Communications*, **1977**, 23, 89-93	1.6	24
14	Neutron Spectroscopy of Naphthalene Crystal Internal Phonon Modes. *Physica Status Solidi (B): Basic Research*, **1976**, 75, 105-116	1.3	21
13	Multiphonon absorption in molecular crystals. *Physica Status Solidi (B): Basic Research*, **1976**, 78, 325-333	1.3	2
12	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-K5	1.3	3
11	Isotopic effect in the absorption spectra of naphthalene crystal. *Chemical Physics*, **1975**, 8, 99-111	2.3	9
10	Exciton-phonon interaction and energy transfer in benzene and isotopically impure deuterobenzene crystals. *Journal of Luminescence*, **1974**, 8, 349-358	3.8	3
9	Spectroscopy of Molecular Crystals: A Bibliography for 1971. *Molecular Crystals and Liquid Crystals*, **1973**, 19, 331-367		1
8	ELECTRON-VIBRATIONAL SPECTRA OF MOLECULES AND CRYSTALS. *Uspekhi Fizicheskikh Nauk*, **1972**, 14, 484-511		28
7	SIXTH ALL-UNION SEMINAR ON "EXCITONS IN CRYSTALS". *Uspekhi Fizicheskikh Nauk*, **1972**, 14, 530-532		
6	Luminescence spectra and adsorption characteristics of naphthalene on various metal-substituted forms of type X zeolite. *Theoretical and Experimental Chemistry*, **1972**, 5, 156-158	1.3	
5	The electronic states of naphthalene molecules adsorbed on a zeolite. *Theoretical and Experimental Chemistry*, **1969**, 3, 220-223	1.3	
4	A New Approach to the Vibronic Spectra of Molecular Crystals. *Physica Status Solidi (B): Basic Research*, **1967**, 19, 395-406	1.3	36
3	Structure of Exciton Bands in Crystalline Anthracene. *Physica Status Solidi (B): Basic Research*, **1965**, 11, 877-890	1.3	50
2	Spin Chemical Physics of Graphene		2