

# Elena Voloshina

## List of Publications by Citations

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109  
papers

2,367  
citations

27  
h-index

45  
g-index

115  
ext. papers

2,593  
ext. citations

4.1  
avg, IF

5.29  
L-index

#	Paper	IF	Citations
109	Induced magnetism of carbon atoms at the graphene/Ni(111) interface. <i>Applied Physics Letters</i> , <b>2010</b> , 96, 012504	3.4	155
108	On the physisorption of water on graphene: a CCSD(T) study. <i>Physical Chemistry Chemical Physics</i> , <b>2011</b> , 13, 12041-7	3.6	152
107	Graphene on metallic surfaces: problems and perspectives. <i>Physical Chemistry Chemical Physics</i> , <b>2012</b> , 14, 13502-14	3.6	144
106	Electronic structure and magnetic properties of the graphene/Fe/Ni(111) intercalation-like system. <i>Physical Chemistry Chemical Physics</i> , <b>2011</b> , 13, 7534-9	3.6	100
105	Structural and electronic properties of the graphene/Al/Ni(111) intercalation system. <i>New Journal of Physics</i> , <b>2011</b> , 13, 113028	2.9	95
104	Photochromism of Spirooxazines in Homogeneous Solution and Phospholipid Liposomes. <i>Journal of the American Chemical Society</i> , <b>1998</b> , 120, 12707-12713	16.4	94
103	Graphene on Rh(111): Scanning tunneling and atomic force microscopies studies. <i>Applied Physics Letters</i> , <b>2012</b> , 100, 241606	3.4	88
102	Electronic structure and imaging contrast of graphene moiré on metals. <i>Scientific Reports</i> , <b>2013</b> , 3, 1072	4.9	80
101	Graphene growth and properties on metal substrates. <i>Journal of Physics Condensed Matter</i> , <b>2015</b> , 27, 303002	1.8	69
100	Understanding the origin of band gap formation in graphene on metals: graphene on Cu/Ir(111). <i>Scientific Reports</i> , <b>2014</b> , 4, 5704	4.9	67
99	Structural and electronic properties of epitaxial multilayer h-BN on Ni(111) for spintronics applications. <i>Scientific Reports</i> , <b>2016</b> , 6, 23547	4.9	67
98	Water adsorption and O-defect formation on FeO(0001) surfaces. <i>Physical Chemistry Chemical Physics</i> , <b>2016</b> , 18, 25560-25568	3.6	61
97	Kinetic and Thermodynamic Investigations of the Photochromism and Solvatochromism of Semipermanent Merocyanines. <i>Journal of Physical Chemistry A</i> , <b>2001</b> , 105, 8417-8422	2.8	48
96	In situ fabrication of quasi-free-standing epitaxial graphene nanoflakes on gold. <i>ACS Nano</i> , <b>2014</b> , 8, 3735-3742	16.7	47
95	Polyketides from the marine-derived fungus <i>Ascochyta salicorniae</i> and their potential to inhibit protein phosphatases. <i>Organic and Biomolecular Chemistry</i> , <b>2006</b> , 4, 2233-40	3.9	44
94	Structural and electronic properties of graphene nanoflakes on Au(111) and Ag(111). <i>Scientific Reports</i> , <b>2016</b> , 6, 23439	4.9	43
93	Embedding procedure for ab initio correlation calculations in group II metals. <i>Journal of Chemical Physics</i> , <b>2007</b> , 126, 134115	3.9	40

92	Restoring a nearly free-standing character of graphene on Ru(0001) by oxygen intercalation. <i>Scientific Reports</i> , <b>2016</b> , 6, 20285	4.9	39
91	Interaction of Pyridine Derivatives with a Gold (111) Surface as a Model for Adsorption to Large Nanoparticles. <i>Journal of Physical Chemistry C</i> , <b>2013</b> , 117, 4470-4479	3.8	36
90	General approach to understanding the electronic structure of graphene on metals. <i>Materials Research Express</i> , <b>2014</b> , 1, 035603	1.7	36
89	Theoretical study on the adsorption of pyridine derivatives on graphene. <i>Chemical Physics Letters</i> , <b>2011</b> , 510, 220-223	2.5	32
88	Theoretical description of X-ray absorption spectroscopy of the graphene-metal interfaces. <i>Journal of Chemical Physics</i> , <b>2013</b> , 138, 154706	3.9	31
87	Decoupling of graphene from Ni(111) via formation of an interfacial NiO layer. <i>Carbon</i> , <b>2017</b> , 121, 10-16	10.4	30
86	Performance of Dispersion-Corrected DFT for the Weak Interaction between Aromatic Molecules and Extended Carbon-Based Systems. <i>Journal of Physical Chemistry C</i> , <b>2015</b> , 119, 1898-1904	3.8	30
85	Communication: A combined periodic density functional and incremental wave-function-based approach for the dispersion-accounting time-resolved dynamics of He nanodroplets on surfaces: He/graphene. <i>Journal of Chemical Physics</i> , <b>2014</b> , 141, 151102	3.9	30
84	Influence of electronic correlations on the ground-state properties of cerium dioxide. <i>Journal of Chemical Physics</i> , <b>2006</b> , 124, 234711	3.9	30
83	First Multireference Correlation Treatment of Bulk Metals. <i>Journal of Chemical Theory and Computation</i> , <b>2014</b> , 10, 1698-706	6.4	28
82	First-principles study of the connection between structure and electronic properties of gallium. <i>Physical Review B</i> , <b>2009</b> , 79,	3.3	26
81	Multichannel scanning probe microscopy and spectroscopy of graphene moiré structures. <i>Physical Chemistry Chemical Physics</i> , <b>2014</b> , 16, 3894-908	3.6	23
80	Scanning probe microscopy and spectroscopy of graphene on metals. <i>Physica Status Solidi (B): Basic Research</i> , <b>2015</b> , 252, 451-468	1.3	23
79	Growth and electronic structure of graphene on semiconducting Ge(110). <i>Carbon</i> , <b>2017</b> , 122, 428-433	10.4	22
78	Graphene on ferromagnetic surfaces and its functionalization with water and ammonia. <i>Nanoscale Research Letters</i> , <b>2011</b> , 6, 214	5	22
77	Electronic, magnetic and optical properties of MnPX (X = S, Se) monolayers with and without chalcogen defects: a first-principles study.. <i>RSC Advances</i> , <b>2020</b> , 10, 851-864	3.7	22
76	The graphene/n-Ge(110) interface: structure, doping, and electronic properties. <i>Nanoscale</i> , <b>2018</b> , 10, 6088-6098	7.7	21
75	Wave-function-based ab initio method for metals: Application of the incremental scheme to magnesium. <i>Physical Review B</i> , <b>2007</b> , 75,	3.3	21

74	Local correlation method for metals: Benchmarks for surface and adsorption energies. <i>Physical Review B</i> , <b>2012</b> , 85,	3.3	20
73	Interaction of Water Molecules with the $\alpha$ -Fe <sub>2</sub> O <sub>3</sub> (0001) Surface: A Combined Experimental and Computational Study. <i>Journal of Physical Chemistry C</i> , <b>2019</b> , 123, 8324-8335	3.8	18
72	Spiropyrans and spirooxazines. 1. Synthesis and photochromic properties of 9"-hydroxy- and 9"-alkoxy-substituted spironaphthooxazines. <i>Russian Chemical Bulletin</i> , <b>2003</b> , 52, 1172-1181	1.7	16
71	Layer-by-Layer Decoupling of Twisted Graphene Sheets Epitaxially Grown on a Metal Substrate. <i>Small</i> , <b>2018</b> , 14, e1703701	11	15
70	Accurate quantum-chemical description of gold complexes with pyridine and its derivatives. <i>Journal of Computational Chemistry</i> , <b>2011</b> , 32, 1839-45	3.5	15
69	An attempt to determine the absolute configuration of two ascolactone stereoisomers with time-dependent density functional theory. <i>Chirality</i> , <b>2006</b> , 18, 413-8	2.1	15
68	Structural and electronic properties of graphene-based junctions for spin-filtering: The graphene/Al/Ni(1 1 1) intercalation-like system. <i>Applied Surface Science</i> , <b>2013</b> , 267, 8-11	6.7	14
67	Structural and electronic properties of Fe <sub>3</sub> O <sub>4</sub> /graphene/Ni(111) junctions. <i>Physica Status Solidi - Rapid Research Letters</i> , <b>2011</b> , 5, 226-228	2.5	14
66	Electronic structure, magnetism, and spin-dependent transport of CeMnNi <sub>4</sub> . <i>Physical Review B</i> , <b>2006</b> , 73,	3.3	13
65	Post-Hartree-Fock studies of the He/Mg(0001) interaction: Anti-corrugation, screening, and pairwise additivity. <i>Journal of Chemical Physics</i> , <b>2016</b> , 144, 244707	3.9	13
64	Adsorption of multivalent alkylthiols on Au(111) surface: insights from DFT. <i>Journal of Computational Chemistry</i> , <b>2014</b> , 35, 204-13	3.5	12
63	Spiropyrans and spirooxazines. <i>Russian Chemical Bulletin</i> , <b>2008</b> , 57, 151-158	1.7	12
62	First Asymmetric Synthesis and Determination of the Absolute Configuration of a Lignan Isolated from <i>Virola sebifera</i> . <i>European Journal of Organic Chemistry</i> , <b>2005</b> , 2005, 1984-1990	3.2	11
61	Conformational Analysis and CD Calculations of Methyl-Substituted 13-Tridecano-13-lactones. <i>Helvetica Chimica Acta</i> , <b>2005</b> , 88, 194-209	2	11
60	Epitaxial graphene/Ge interfaces: a minireview. <i>Nanoscale</i> , <b>2020</b> , 12, 11416-11426	7.7	10
59	Determination of the absolute configuration of calliactine by quantum chemical calculations. <i>International Journal of Quantum Chemistry</i> , <b>2004</b> , 100, 1104-1113	2.1	10
58	Spiropyrans and spirooxazines. 2. Synthesis, structures, and photochromic properties of 6"-cyano-substituted spironaphthooxazines. <i>Russian Chemical Bulletin</i> , <b>2003</b> , 52, 2038-2047	1.7	10
57	On the application of the incremental scheme to ionic solids: test of different embeddings. <i>Theoretical Chemistry Accounts</i> , <b>2005</b> , 114, 259-264	1.9	10

56	Spectroscopic and DFT studies of graphene intercalation systems on metals. <i>Journal of Electron Spectroscopy and Related Phenomena</i> , <b>2017</b> , 219, 77-85	1.7	9
55	Adsorption of NO <sub>2</sub> on WSe <sub>2</sub> : DFT and photoelectron spectroscopy studies. <i>Journal of Physics Condensed Matter</i> , <b>2016</b> , 28, 364003	1.8	9
54	Atomic force spectroscopy and density-functional study of graphene corrugation on Ru(0001). <i>Physical Review B</i> , <b>2016</b> , 93,	3.3	9
53	Development of a Wavefunction-based Ab Initio Method for Metals Applying the Method of Increments. <i>Zeitschrift Fur Physikalische Chemie</i> , <b>2010</b> , 224, 369-381	3.1	9
52	Correlation energies for small magnesium clusters in comparison with bulk magnesium. <i>Molecular Physics</i> , <b>2007</b> , 105, 2849-2855	1.7	9
51	Cohesive properties of CeN and LaN from first principles. <i>Journal of Computational Chemistry</i> , <b>2008</b> , 29, 2107-12	3.5	9
50	Photochromic properties of six 5-O-n-alkyl,6?-CN substituted spironaphthoxazines. <i>International Journal of Photoenergy</i> , <b>2004</b> , 6, 199-204	2.1	9
49	Correlations in the Electronic Structure of van der Waals NiPS Crystals: An X-ray Absorption and Resonant Photoelectron Spectroscopy Study. <i>Journal of Physical Chemistry Letters</i> , <b>2021</b> , 12, 2400-2405	6.4	9
48	Dirac Fermions in Half-Metallic Ferromagnetic Mixed Cr <sub>1-x</sub> MxPSe <sub>3</sub> Monolayers. <i>Advanced Theory and Simulations</i> , <b>2020</b> , 3, 2000228	3.5	8
47	Ab initio investigation of ground-state properties of group-12 fluorides. <i>International Journal of Quantum Chemistry</i> , <b>2014</b> , 114, 943-951	2.1	8
46	Quantum-chemical approach to cohesive properties of metallic beryllium. <i>Journal of Physics: Conference Series</i> , <b>2008</b> , 117, 012029	0.3	8
45	Spiropyrans and spirooxazines. 3. Synthesis of photochromic 5?-(4,5-diphenyl-1,3-oxazol-2-yl)-spiro[indoline-2,3?-naphtho[2,3-b]pyran]. <i>Russian Chemical Bulletin</i> , <b>2005</b> , 54, 705-710	1.7	8
44	Unoccupied electronic band structure of pentagonal Si nanoribbons on Ag(110). <i>Physical Chemistry Chemical Physics</i> , <b>2019</b> , 21, 17811-17820	3.6	7
43	Graphene on Rh(111): Combined DFT, STM, and NC-AFM Studies. <i>Procedia Engineering</i> , <b>2014</b> , 93, 8-16		7
42	Dual character of excited charge carriers in graphene on Ni(111). <i>Physical Review B</i> , <b>2014</b> , 89,	3.3	7
41	Realistic Large-Scale Modeling of Rashba and Induced Spin-Orbit Effects in Graphene/High-Z-Metal Systems. <i>Advanced Theory and Simulations</i> , <b>2018</b> , 1, 1800063	3.5	6
40	The role of electron correlations in the binding properties of Ca, Sr, and Ba. <i>Journal of Physics Condensed Matter</i> , <b>2010</b> , 22, 275504	1.8	6
39	To the synthesis and characterization of layered metal phosphorus triselenides proposed for electrochemical sensing and energy applications. <i>Chemical Physics Letters</i> , <b>2020</b> , 754, 137627	2.5	5

38	Electronic and Magnetic Properties of the Graphene/Eu/Ni(111) Hybrid System. <i>Zeitschrift Fur Naturforschung - Section A Journal of Physical Sciences</i> , <b>2014</b> , 69, 297-302	1.4	5
37	Specific many-electron effects in X-ray spectra of simple metals and graphene. <i>Physical Chemistry Chemical Physics</i> , <b>2013</b> , 15, 6749-56	3.6	5
36	Ferromagnetic coupling in EuCd(0001) observed by spin-resolved photoelectron spectroscopy. <i>Physical Review B</i> , <b>2006</b> , 73,	3.3	5
35	Adsorption of water on the pristine and defective semiconducting 2D CrP monolayers (S, Se). <i>Journal of Physics Condensed Matter</i> , <b>2021</b> , 33,	1.8	5
34	Local electronic properties of the graphene-protected giant Rashba-split BiAg <sub>2</sub> surface. <i>Physical Review B</i> , <b>2017</b> , 95,	3.3	4
33	Dirac Electron Behavior for Spin-Up Electrons in Strongly Interacting Graphene on Ferromagnetic MnGe. <i>Journal of Physical Chemistry Letters</i> , <b>2019</b> , 10, 3212-3216	6.4	4
32	Polarographic and spectrophotometric studies of the spiro[indolin-pyridobenzopyrane] complexes with the heavy metal ions. <i>Russian Journal of General Chemistry</i> , <b>2009</b> , 79, 1191-1196	0.7	4
31	Observation of surface state on ultrathin fcc $\overline{\Gamma}$ Mn(1 1 1) layer. <i>Surface Science</i> , <b>2006</b> , 600, 4328-4331	1.8	4
30	To Estimation of pKa for Spiroprans of the Indoline Series. <i>Russian Journal of General Chemistry</i> , <b>2002</b> , 72, 1468-1472	0.7	4
29	Mott-Hubbard insulating state for the layered van der Waals [Formula: see text] (X: S, Se) as revealed by NEXAFS and resonant photoelectron spectroscopy.. <i>Scientific Reports</i> , <b>2022</b> , 12, 735	4.9	4
28	Adsorption of Water Molecules on Pristine and Defective NiPX <sub>3</sub> (X: S, Se) Monolayers. <i>Advanced Theory and Simulations</i> , <b>2021</b> , 4, 2100182	3.5	4
27	Realization of the electric-field driven $\overline{\Gamma}$ ne-material-based magnetic tunnel junction using van der Waals antiferromagnetic MnPX <sub>3</sub> (X: S, Se). <i>Journal of Materials Chemistry C</i> , <b>2022</b> , 10, 3812-3818	7.1	4
26	Electronic Structure and Magnetic Properties of Graphene/Ni <sub>3</sub> Mn/Ni(111) Trilayer. <i>Journal of Physical Chemistry C</i> , <b>2019</b> , 123, 4994-5002	3.8	3
25	Intercalation of O <sub>2</sub> and N <sub>2</sub> in the Graphene/Ni Interfaces of Different Morphologies. <i>Journal of Physical Chemistry C</i> , <b>2019</b> , 123, 16137-16145	3.8	3
24	Quantum Well States for Graphene Spin-Texture Engineering. <i>Journal of Physical Chemistry Letters</i> , <b>2020</b> , 11, 1594-1600	6.4	3
23	Wavefunction-based ab initio correlation method for metals: application of the incremental scheme to Be, Mg, Zn, Cd, and Hg. <i>Chemical Modelling</i> , 162-209	2	3
22	(E)-4-Methyl-1-tributylstannyl-oct-1-en-6-yn-3-ol: Circular Dichroism Measurement and Determination of the Absolute Configuration by Quantum-chemical CD Calculations. <i>Zeitschrift Fur Naturforschung - Section A Journal of Physical Sciences</i> , <b>2004</b> , 59, 124-132	1.4	3
21	Intercalation of Mn in graphene/Cu(111) interface: insights to the electronic and magnetic properties from theory. <i>Scientific Reports</i> , <b>2020</b> , 10, 21684	4.9	3

20	Graphene Layer Morphology as an Indicator of the Metal Alloy Formation at the Interface. <i>Journal of Physical Chemistry Letters</i> , <b>2021</b> , 12, 19-25	6.4	3
19	Impact of the metal substrate on the electronic structure of armchair graphene nanoribbons. <i>Chemical Physics Letters</i> , <b>2014</b> , 597, 148-152	2.5	2
18	Calculation of the X-Ray emission K and L 2,3 bands of metallic magnesium and aluminum with allowance for multielectron effects. <i>Journal of Experimental and Theoretical Physics</i> , <b>2014</b> , 118, 11-17	1	2
17	Comment on "Spin-Orbit Coupling Induced Gap in Graphene on Pt(111) with Intercalated Pb Monolayer". <i>ACS Nano</i> , <b>2017</b> , 11, 10627-10629	16.7	2
16	Electronic and Magnetic Properties of the Graphene- Ferromagnet Interfaces: Theory vs. Experiment <b>2011</b> ,		2
15	Preparation and photoemission investigation of bulklike $\delta$ Mn films on W(110). <i>Physical Review B</i> , <b>2010</b> , 81,	3.3	2
14	Influence of surface and subsurface Co $\Gamma$ alloy on the electronic properties of graphene. <i>Carbon</i> , <b>2021</b> , 183, 251-258	10.4	2
13	Topological Quasi-2D Semimetal CoSnS: Insights into Electronic Structure from NEXAFS and Resonant Photoelectron Spectroscopy. <i>Journal of Physical Chemistry Letters</i> , <b>2021</b> , 12, 9807-9811	6.4	2
12	A study of spiro[indoline-pyridobenzopyrans] by differential pulse voltammetry on a dropping mercury electrode and quantum chemistry. <i>Russian Journal of General Chemistry</i> , <b>2008</b> , 78, 662-667	0.7	1
11	Modification of the Magnetic and Electronic Properties of the Graphene-Ni(111) Interface via Halogens Intercalation. <i>Advanced Theory and Simulations</i> , 2100319	3.5	1
10	-Chloridolithates from Ionothermal Synthesis. <i>Inorganic Chemistry</i> , <b>2021</b> ,	5.1	1
9	Development of a Wavefunction-based Ab Initio Method for Metals Applying the Method of Increments <b>2010</b> , 79-91		0
8	Second Floor of Flatland: Epitaxial Growth of Graphene on Hexagonal Boron Nitride. <i>Small</i> , <b>2021</b> , 17, e2102747	11	0
7	Hematite, Its Stable Surface Terminations and Their Reactivity Toward Water <b>2018</b> , 115-121		0
6	Electronic and Magnetic Properties of the Graphene/Y/Co(0001) Interfaces: Insights from the Density Functional Theory Analysis.. <i>ACS Omega</i> , <b>2022</b> , 7, 7304-7310	3.9	0
5	New formyl-substituted spiropyranes of the indoline series. <i>Chemistry of Heterocyclic Compounds</i> , <b>1997</b> , 32, 1427-1428	1.4	
4	Spin-resolved photoelectron spectroscopy of rare-earth overlayers on rare-earth and d-metal substrates. <i>Journal of Magnetism and Magnetic Materials</i> , <b>2008</b> , 320, e231-e234	2.8	
3	Graphene Properties on Metals <b>2018</b> , 138-144		

- 2 Second Floor of Flatland: Epitaxial Growth of Graphene on Hexagonal Boron Nitride (Small 36/2021). *Small*, **2021**, 17, 2170188 11
- 1 Electronic and Magnetic Properties of The Graphene/RE/Ni(111) (RE: La, Yb) Intercalation-Like Interfaces: A DFT Analysis. *Advanced Theory and Simulations*, 2100621 3-5