Elena Voloshina

List of Publications by Year
in descending order

112 papers	2,797 citations	185998 28 h-index	197535 49 g-index
115 all docs	115 docs citations	115 times ranked	3798 citing authors

#	Article	IF	Citations
1	On the physisorption of water on graphene: a CCSD(T) study. Physical Chemistry Chemical Physics, 2011, 13, 12041.	1.3	172
2	Induced magnetism of carbon atoms at the graphene/Ni(111) interface. Applied Physics Letters, 2010, 96, .	1.5	169
3	Graphene on metallic surfaces: problems and perspectives. Physical Chemistry Chemical Physics, 2012, 14, 13502.	1.3	157
4	Electronic structure and magnetic properties of the graphene/Fe/Ni(111) intercalation-like system. Physical Chemistry Chemical Physics, 2011, 13, 7534.	1.3	110
5	Photochromism of Spirooxazines in Homogeneous Solution and Phospholipid Liposomes. Journal of the American Chemical Society, 1998, 120, 12707-12713.	6.6	104
6	Structural and electronic properties of the graphene/Al/Ni(111) intercalation system. New Journal of Physics, 2011, 13, 113028.	1.2	103
7	Graphene on Rh(111): Scanning tunneling and atomic force microscopies studies. Applied Physics Letters, 2012, 100, .	1.5	99
8	Water adsorption and O-defect formation on Fe₂O₃(0001) surfaces. Physical Chemistry Chemical Physics, 2016, 18, 25560-25568.	1.3	91
9	Graphene growth and properties on metal substrates. Journal of Physics Condensed Matter, 2015, 27, 303002.	0.7	86
10	Electronic structure and imaging contrast of graphene moirÃ© on metals. Scientific Reports, 2013, 3, 1072.	1.6	85
11	Structural and electronic properties of epitaxial multilayer h-BN on Ni(111) for spintronics applications. Scientific Reports, 2016, 6, 23547.	1.6	80
12	Understanding the origin of band gap formation in graphene on metals: graphene on Cu/Ir(111). Scientific Reports, 2015, 4, 5704.	1.6	74
13	Electronic, magnetic and optical properties of MnPX₃ (X = S, Se) monolayers with and without chalcogen defects: a first-principles study. RSC Advances, 2020, 10, 851-864.	1.7	57
14	Kinetic and Thermodynamic Investigations of the Photochromism and Solvatochromism of Semipermanent Merocyanines. Journal of Physical Chemistry A, 2001, 105, 8417-8422.	1.1	52
15	Structural and electronic properties of graphene nanoflakes on Au(111) and Ag(111). Scientific Reports, 2016, 6, 23439.	1.6	51
16	In Situ Fabrication Of Quasi-Free-Standing Epitaxial Graphene Nanoflakes On Gold. ACS Nano, 2014, 8, 3735-3742.	7.3	50
17	Polyketides from the marine-derived fungus Ascochyta salicorniae and their potential to inhibit protein phosphatases. Organic and Biomolecular Chemistry, 2006, 4, 2233-2240.	1.5	49
18	Restoring a nearly free-standing character of graphene on Ru(0001) by oxygen intercalation. Scientific Reports, 2016, 6, 20285.	1.6	46

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19	Interaction of Pyridine Derivatives with a Gold (111) Surface as a Model for Adsorption to Large Nanoparticles. Journal of Physical Chemistry C, 2013, 117, 4470-4479.	1.5	45
20	General approach to understanding the electronic structure of graphene on metals. Materials Research Express, 2014, 1, 035603.	0.8	43
21	Embedding procedure for ab initio correlation calculations in group II metals. Journal of Chemical Physics, 2007, 126, 134115.	1.2	42
22	Theoretical study on the adsorption of pyridine derivatives on graphene. Chemical Physics Letters, 2011, 510, 220-223.	1.2	39
23	Performance of Dispersion-Corrected DFT for the Weak Interaction between Aromatic Molecules and Extended Carbon-Based Systems. Journal of Physical Chemistry C, 2015, 119, 1898-1904.	1.5	37
24	Communication: A combined periodic density functional and incremental wave-function-based approach for the dispersion-accounting time-resolved dynamics of 4He nanodroplets on surfaces: 4He/graphene. Journal of Chemical Physics, 2014, 141, 151102.	1.2	34
25	Decoupling of graphene from Ni(111) via formation of an interfacial NiO layer. Carbon, 2017, 121, 10-16.	5.4	34
26	Theoretical description of X-ray absorption spectroscopy of the graphene-metal interfaces. Journal of Chemical Physics, 2013, 138, 154706.	1.2	33
27	Influence of electronic correlations on the ground-state properties of cerium dioxide. Journal of Chemical Physics, 2006, 124, 234711.	1.2	30
28	First Multireference Correlation Treatment of Bulk Metals. Journal of Chemical Theory and Computation, 2014, 10, 1698-1706.	2.3	30
29	First-principles study of the connection between structure and electronic properties of gallium. Physical Review B, 2009, 79, .	1.1	28
30	Graphene on ferromagnetic surfaces and its functionalization with water and ammonia. Nanoscale Research Letters, 2011, 6, 214.	3.1	28
31	The graphene/n-Ge(110) interface: structure, doping, and electronic properties. Nanoscale, 2018, 10, 6088-6098.	2.8	28
32	Interaction of Water Molecules with the Î±-Fe₂O₃(0001) Surface: A Combined Experimental and Computational Study. Journal of Physical Chemistry C, 2019, 123, 8324-8335.	1.5	26
33	Growth and electronic structure of graphene on semiconducting Ge(110). Carbon, 2017, 122, 428-433.	5.4	25
34	Multichannel scanning probe microscopy and spectroscopy of graphene moirÃ© structures. Physical Chemistry Chemical Physics, 2014, 16, 3894.	1.3	24
35	Scanning probe microscopy and spectroscopy of graphene on metals. Physica Status Solidi (B): Basic Research, 2015, 252, 451-468.	0.7	23
36	Epitaxial graphene/Ge interfaces: a minireview. Nanoscale, 2020, 12, 11416-11426.	2.8	22

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37	Wave-function-basedab initiomethod for metals: Application of the incremental scheme to magnesium. Physical Review B, 2007, 75, .	1.1	21
38	Local correlation method for metals: Benchmarks for surface and adsorption energies. Physical Review B, 2012, 85, .	1.1	21
39	Correlations in the Electronic Structure of van der Waals NiPS₃ Crystals: An X-ray Absorption and Resonant Photoelectron Spectroscopy Study. Journal of Physical Chemistry Letters, 2021, 12, 2400-2405.	2.1	21
40	Title is missing!. Russian Chemical Bulletin, 2003, 52, 1172-1181.	0.4	18
41	Dirac Fermions in Halfâ€Metallic Ferromagnetic Mixed Cr1â^'xM_xPSe₃ Monolayers. Advanced Theory and Simulations, 2020, 3, 2000228.	1.3	18
42	Layerâ€byâ€Layer Decoupling of Twisted Graphene Sheets Epitaxially Grown on a Metal Substrate. Small, 2018, 14, e1703701.	5.2	17
43	Spiropyrans and spirooxazines. Russian Chemical Bulletin, 2008, 57, 151-158.	0.4	16
44	Structural and electronic properties of Fe₃O₄/graphene/Ni(111) junctions. Physica Status Solidi - Rapid Research Letters, 2011, 5, 226-228.	1.2	16
45	Accurate quantumâ€chemical description of gold complexes with pyridine and its derivatives. Journal of Computational Chemistry, 2011, 32, 1839-1845.	1.5	16
46	Post-Hartree-Fock studies of the He/Mg(0001) interaction: Anti-corrugation, screening, and pairwise additivity. Journal of Chemical Physics, 2016, 144, 244707.	1.2	16
47	An attempt to determine the absolute configuration of two ascolactone stereoisomers with time-dependent density functional theory. Chirality, 2006, 18, 413-418.	1.3	15
48	Structural and electronic properties of graphene-based junctions for spin-filtering: The graphene/Al/Ni(111) intercalation-like system. Applied Surface Science, 2013, 267, 8-11.	3.1	14
49	Electronic structure, magnetism, and spin-dependent transport ofCeMnNi4. Physical Review B, 2006, 73, .	1.1	13
50	Mottâ€“Hubbard insulating state for the layered van der Waals $$hbox {FePX}_3$$ (X: S, Se) as revealed by NEXAFS and resonant photoelectron spectroscopy. Scientific Reports, 2022, 12, 735.	1.6	13
51	On the application of the incremental scheme to ionic solids: test of different embeddings. Theoretical Chemistry Accounts, 2005, 114, 259-264.	0.5	12
52	Adsorption of multivalent alkylthiols on Au(111) surface: Insights from DFT. Journal of Computational Chemistry, 2014, 35, 204-213.	1.5	12
53	Adsorption of NO₂on WSe₂: DFT and photoelectron spectroscopy studies. Journal of Physics Condensed Matter, 2016, 28, 364003.	0.7	12
54	Spectroscopic and DFT studies of graphene intercalation systems on metals. Journal of Electron Spectroscopy and Related Phenomena, 2017, 219, 77-85.	0.8	12

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55	To the synthesis and characterization of layered metal phosphorus triselenides proposed for electrochemical sensing and energy applications. Chemical Physics Letters, 2020, 754, 137627.	1.2	12
56	Spiropyrans and spirooxazines. 2. Synthesis, structures, and photochromic properties of 6"-cyano-substituted spironaphthooxazines. Russian Chemical Bulletin, 2003, 52, 2038-2047.	0.4	11
57	Determination of the absolute configuration of calliactine by quantum chemical calculations. International Journal of Quantum Chemistry, 2004, 100, 1104-1113.	1.0	11
58	First Asymmetric Synthesis and Determination of the Absolute Configuration of a Lignan Isolated fromVirola sebifera. European Journal of Organic Chemistry, 2005, 2005, 1984-1990.	1.2	11
59	Conformational Analysis and CD Calculations of Methyl-Substituted 13-Tridecano-13-lactones. Helvetica Chimica Acta, 2005, 88, 194-209.	1.0	11
60	Correlation energies for small magnesium clusters in comparison with bulk magnesium. Molecular Physics, 2007, 105, 2849-2855.	0.8	11
61	Realistic Largeâ€Scale Modeling of Rashba and Induced Spinâ€“Orbit Effects in Graphene/Highâ€Zâ€Metal Systems. Advanced Theory and Simulations, 2018, 1, 1800063.	1.3	11
62	To Estimation of pKa for Spiropyrans of the Indoline Series. Russian Journal of General Chemistry, 2002, 72, 1468-1472.	0.3	10
63	Photochromic properties of six 5-O-n-alkyl,6â€²-CN substituted spironaphthoxazines. International Journal of Photoenergy, 2004, 6, 199-204.	1.4	10
64	Spiropyrans and spirooxazines. 3. Synthesis of photochromic 5â€²-(4,5-diphenyl-1,3-oxazol-2-yl)-spiro[indoline-2,3â€²-naphtho[2,3-b]pyran]. Russian Chemical Bulletin, 2005, 54, 705-710.	0.4	10
65	Cohesive properties of CeN and LaN from first principles. Journal of Computational Chemistry, 2008, 29, 2107-2112.	1.5	10
66	Development of a Wavefunction-based Ab Initio Method for Metals Applying the Method of Increments. Zeitschrift Fur Physikalische Chemie, 2010, 224, 369-381.	1.4	10
67	Atomic force spectroscopy and density-functional study of graphene corrugation on Ru(0001). Physical Review B, 2016, 93, .	1.1	10
68	Adsorption of water on the pristine and defective semiconducting 2D CrPX3 monolayers (X: S, Se). Journal of Physics Condensed Matter, 2021, 33, .	0.7	10
69	Realization of the electric-field driven â€œone-materialâ€•based magnetic tunnel junction using van der Waals antiferromagnetic MnPX₃ (X: S, Se). Journal of Materials Chemistry C, 2022, 10, 3812-3818.	2.7	10
70	Quantum-chemical approach to cohesive properties of metallic beryllium. Journal of Physics: Conference Series, 2008, 117, 012029.	0.3	9
71	Ab initio investigation of groundâ€state properties of groupâ€12 fluorides. International Journal of Quantum Chemistry, 2014, 114, 943-951.	1.0	9
72	Unoccupied electronic band structure of pentagonal Si nanoribbons on Ag(110). Physical Chemistry Chemical Physics, 2019, 21, 17811-17820.	1.3	9

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73	Graphene on Rh(111): Combined DFT, STM, and NC-AFM Studies. Procedia Engineering, 2014, 93, 8-16.	1.2	8
74	Adsorption of Water Molecules on Pristine and Defective NiPX₃ (X: S, Se) Monolayers. Advanced Theory and Simulations, 2021, 4, 2100182.	1.3	8
75	Dual character of excited charge carriers in graphene on Ni(111). Physical Review B, 2014, 89, .	1.1	7
76	Dirac Electron Behavior for Spin-Up Electrons in Strongly Interacting Graphene on Ferromagnetic Mn₅Ge₃. Journal of Physical Chemistry Letters, 2019, 10, 3212-3216.	2.1	7
77	The role of electron correlations in the binding properties of Ca, Sr, and Ba. Journal of Physics Condensed Matter, 2010, 22, 275504.	0.7	6
78	Specific many-electron effects in X-ray spectra of simple metals and graphene. Physical Chemistry Chemical Physics, 2013, 15, 6749.	1.3	6
79	Intercalation of Mn in graphene/Cu(111) interface: insights to the electronic and magnetic properties from theory. Scientific Reports, 2020, 10, 21684.	1.6	6
80	Ferromagnetic coupling inEuâˆ•Gd(0001)observed by spin-resolved photoelectron spectroscopy. Physical Review B, 2006, 73, .	1.1	5
81	Electronic and Magnetic Properties of the Graphene/Eu/Ni(111) Hybrid System. Zeitschrift Fur Naturforschung - Section A Journal of Physical Sciences, 2014, 69, 297-302.	0.7	5
82	Quantum Well States for Graphene Spin-Texture Engineering. Journal of Physical Chemistry Letters, 2020, 11, 1594-1600.	2.1	5
83	Observation of surface state on ultrathin fcc Î³-Mn(111) layer. Surface Science, 2006, 600, 4328-4331.	0.8	4
84	Polarographic and spectrophotometric studies of the spiro[indolin-pyridobenzopyrane] complexes with the heavy metal ions. Russian Journal of General Chemistry, 2009, 79, 1191-1196.	0.3	4
85	Electronic and Magnetic Properties of the Graphene- Ferromagnet Interfaces: Theory vs. Experiment. , 2011, , .		4
86	Impact of the metal substrate on the electronic structure of armchair graphene nanoribbons. Chemical Physics Letters, 2014, 597, 148-152.	1.2	4
87	Local electronic properties of the graphene-protected giant Rashba-split <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mi>BiAg</mml:mi><mml:mn>2</mml:mn></mml:msub></mml:math> surface. Physical Review B, 2017, 95, .	1.1	4
88	Hematite, Its Stable Surface Terminations and Their Reactivity Toward Water. , 2018, , 115-121.		4
89	Graphene Layer Morphology as an Indicator of the Metal Alloy Formation at the Interface. Journal of Physical Chemistry Letters, 2021, 12, 19-25.	2.1	4
90	Topological Quasi-2D Semimetal Co₃Sn₂S₂: Insights into Electronic Structure from NEXAFS and Resonant Photoelectron Spectroscopy. Journal of Physical Chemistry Letters, 2021, 12, 9807-9811.	2.1	4

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91	(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. Zeitschrift Fur Naturforschung - Section A Journal of Physical Sciences, 2004, 59, 124-132.	0.7	3
92	Electronic Structure and Magnetic Properties of Graphene/Ni₃Mn/Ni(111) Trilayer. Journal of Physical Chemistry C, 2019, 123, 4994-5002.	1.5	3
93	Intercalation of O₂ and N₂ in the Graphene/Ni Interfaces of Different Morphologies. Journal of Physical Chemistry C, 2019, 123, 16137-16145.	1.5	3
94	Preparation and photoemission investigation of bulklikeÎ±-Mnfilms on W(110). Physical Review B, 2010, 81, .	1.1	2
95	Calculation of the X-Ray emission K and L 2,3 bands of metallic magnesium and aluminum with allowance for multielectron effects. Journal of Experimental and Theoretical Physics, 2014, 118, 11-17.	0.2	2
96	Comment on â€œSpinâ€“Orbit Coupling Induced Gap in Graphene on Pt(111) with Intercalated Pb Monolayerâ€. ACS Nano, 2017, 11, 10627-10629.	7.3	2
97	Influence of surface and subsurface Coâ€“Ir alloy on the electronic properties of graphene. Carbon, 2021, 183, 251-258.	5.4	2
98	New formyl-substituted spiropyrans of the indoline series. Chemistry of Heterocyclic Compounds, 1997, 32, 1427-1428.	0.6	1
99	A study of spiro[indoline-pyridobenzopyrans] by differential pulse voltammetry on a dropping mercury electrode and quantum chemistry. Russian Journal of General Chemistry, 2008, 78, 662-667.	0.3	1
100	Second Floor of Flatland: Epitaxial Growth of Graphene on Hexagonal Boron Nitride. Small, 2021, 17, 2102747.	5.2	1
101	Development of a Wavefunction-basedAb InitioMethod for Metals Applying the Method of Increments. , 2010, , 79-91.		1
102	Modification of the Magnetic and Electronic Properties of the Grapheneâ€Ni(111) Interface via Halogens Intercalation. Advanced Theory and Simulations, 0, , 2100319.	1.3	1
103	Ino-Chloridolithates from Ionothermal Synthesis. Inorganic Chemistry, 2021, 60, 19145-19151.	1.9	1
104	Electronic and Magnetic Properties of the Graphene/Y/Co(0001) Interfaces: Insights from the Density Functional Theory Analysis. ACS Omega, 2022, 7, 7304-7310.	1.6	1
105	Electronic and Magnetic Properties of The Graphene/RE/Ni(111) (RE: La, Yb) Intercalationâ€Like Interfaces: A DFT Analysis. Advanced Theory and Simulations, 0, , 2100621.	1.3	1
106	Spiropyrans and Spirooxazines. Part 1. Synthesis and Photochromic Properties of 9â€²-Hydroxy- and 9â€²-Alkoxy-Substituted Spironaphthooxazines.. ChemInform, 2004, 35, no.	0.1	0
107	Spiropyrans and Spirooxazines. Part 2. Synthesis, Structures, and Photochromic Properties of 6â€²-Cyano-Substituted Spironaphthooxazines.. ChemInform, 2004, 35, no.	0.1	0
108	Electron-Correlation Effects in Metals from First Principles: a Multi-Reference Incremental Scheme. AIP Conference Proceedings, 2007, , .	0.3	0

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109	Spin-resolved photoelectron spectroscopy of rare-earth overlayers on rare-earth and d-metal substrates. Journal of Magnetism and Magnetic Materials, 2008, 320, e231-e234.	1.0	0
110	Graphene Properties on Metals. , 2018, , 138-144.		0
111	Spintronics: Realistic Large-Scale Modeling of Rashba and Induced Spin-Orbit Effects in Graphene/High-Z-Metal Systems (Adv. Theory Simul. 10/2018). Advanced Theory and Simulations, 2018, 1, 1870028.	1.3	0
112	Second Floor of Flatland: Epitaxial Growth of Graphene on Hexagonal Boron Nitride (Small 36/2021). Small, 2021, 17, 2170188.	5.2	0