Elena Voloshina

List of Publications by Year in Descending Order

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	Mott-Hubbard insulating state for the layered van der Waals [Formula: see text] (X: S, Se) as revealed by NEXAFS and resonant photoelectron spectroscopy.. *Scientific Reports*, **2022**, 12, 735	4.9	4
108	Realization of the electric-field driven one-material-based magnetic tunnel junction using van der Waals antiferromagnetic MnPX3 (X: S, Se). *Journal of Materials Chemistry C*, **2022**, 10, 3812-3818	7.1	4
107	Electronic and Magnetic Properties of the Graphene/Y/Co(0001) Interfaces: Insights from the Density Functional Theory Analysis.. *ACS Omega*, **2022**, 7, 7304-7310	3.9	0
106	Adsorption of Water Molecules on Pristine and Defective NiPX3 (X: S, Se) Monolayers. *Advanced Theory and Simulations*, **2021**, 4, 2100182	3.5	4
105	Correlations in the Electronic Structure of van der Waals NiPS Crystals: An X-ray Absorption and Resonant Photoelectron Spectroscopy Study. *Journal of Physical Chemistry Letters*, **2021**, 12, 2400-2405	6.4	9
104	Adsorption of water on the pristine and defective semiconducting 2D CrPmonolayers (: S, Se). *Journal of Physics Condensed Matter*, **2021**, 33,	1.8	5
103	Second Floor of Flatland: Epitaxial Growth of Graphene on Hexagonal Boron Nitride. *Small*, **2021**, 17, e2102747	11	0
102	Graphene Layer Morphology as an Indicator of the Metal Alloy Formation at the Interface. *Journal of Physical Chemistry Letters*, **2021**, 12, 19-25	6.4	3
101	Second Floor of Flatland: Epitaxial Growth of Graphene on Hexagonal Boron Nitride (Small 36/2021). *Small*, **2021**, 17, 2170188	11	
100	Influence of surface and subsurface Co alloy on the electronic properties of graphene. *Carbon*, **2021**, 183, 251-258	10.4	2
99	Topological Quasi-2D Semimetal CoSnS: Insights into Electronic Structure from NEXAFS and Resonant Photoelectron Spectroscopy. *Journal of Physical Chemistry Letters*, **2021**, 12, 9807-9811	6.4	2
98	-Chloridolithates from Ionothermal Synthesis. *Inorganic Chemistry*, **2021**,	5.1	1
97	Dirac Fermions in Half-Metallic Ferromagnetic Mixed Cr1MxPSe3 Monolayers. *Advanced Theory and Simulations*, **2020**, 3, 2000228	3.5	8
96	Epitaxial graphene/Ge interfaces: a minireview. *Nanoscale*, **2020**, 12, 11416-11426	7.7	10
95	To the synthesis and characterization of layered metal phosphorus triselenides proposed for electrochemical sensing and energy applications. *Chemical Physics Letters*, **2020**, 754, 137627	2.5	5
94	Quantum Well States for Graphene Spin-Texture Engineering. *Journal of Physical Chemistry Letters*, **2020**, 11, 1594-1600	6.4	3
93	Electronic, magnetic and optical properties of MnPX (X = S, Se) monolayers with and without chalcogen defects: a first-principles study.. *RSC Advances*, **2020**, 10, 851-864	3.7	22

92	Intercalation of Mn in graphene/Cu(111) interface: insights to the electronic and magnetic properties from theory. *Scientific Reports*, **2020**, 10, 21684	4.9	3
91	Electronic Structure and Magnetic Properties of Graphene/Ni3Mn/Ni(111) Trilayer. *Journal of Physical Chemistry C*, **2019**, 123, 4994-5002	3.8	3
90	Intercalation of O2 and N2 in the Graphene/Ni Interfaces of Different Morphologies. *Journal of Physical Chemistry C*, **2019**, 123, 16137-16145	3.8	3
89	Dirac Electron Behavior for Spin-Up Electrons in Strongly Interacting Graphene on Ferromagnetic MnGe. *Journal of Physical Chemistry Letters*, **2019**, 10, 3212-3216	6.4	4
88	Unoccupied electronic band structure of pentagonal Si nanoribbons on Ag(110). *Physical Chemistry Chemical Physics*, **2019**, 21, 17811-17820	3.6	7
87	Interaction of Water Molecules with the □Fe2O3(0001) Surface: A Combined Experimental and Computational Study. *Journal of Physical Chemistry C*, **2019**, 123, 8324-8335	3.8	18
86	The graphene/n-Ge(110) interface: structure, doping, and electronic properties. *Nanoscale*, **2018**, 10, 6088-6098	7.7	21
85	Layer-by-Layer Decoupling of Twisted Graphene Sheets Epitaxially Grown on a Metal Substrate. *Small*, **2018**, 14, e1703701	11	15
84	Realistic Large-Scale Modeling of Rashba and Induced Spin□Orbit Effects in Graphene/High-Z-Metal Systems. *Advanced Theory and Simulations*, **2018**, 1, 1800063	3.5	6
83	Graphene Properties on Metals **2018**, 138-144		
82	Hematite, Its Stable Surface Terminations and Their Reactivity Toward Water **2018**, 115-121		0
81	Decoupling of graphene from Ni(111) via formation of an interfacial NiO layer. *Carbon*, **2017**, 121, 10-16	10.4	30
80	Spectroscopic and DFT studies of graphene intercalation systems on metals. *Journal of Electron Spectroscopy and Related Phenomena*, **2017**, 219, 77-85	1.7	9
79	Local electronic properties of the graphene-protected giant Rashba-split BiAg2 surface. *Physical Review B*, **2017**, 95,	3.3	4
78	Comment on "Spin-Orbit Coupling Induced Gap in Graphene on Pt(111) with Intercalated Pb Monolayer". *ACS Nano*, **2017**, 11, 10627-10629	16.7	2
77	Growth and electronic structure of graphene on semiconducting Ge(110). *Carbon*, **2017**, 122, 428-433	10.4	22
76	Water adsorption and O-defect formation on FeO(0001) surfaces. *Physical Chemistry Chemical Physics*, **2016**, 18, 25560-25568	3.6	61
75	Structural and electronic properties of graphene nanoflakes on Au(111) and Ag(111). *Scientific Reports*, **2016**, 6, 23439	4.9	43

74	Adsorption of NO2 on WSe2: DFT and photoelectron spectroscopy studies. *Journal of Physics Condensed Matter*, **2016**, 28, 364003	1.8	9
73	Atomic force spectroscopy and density-functional study of graphene corrugation on Ru(0001). *Physical Review B*, **2016**, 93,	3.3	9
72	Structural and electronic properties of epitaxial multilayer h-BN on Ni(111) for spintronics applications. *Scientific Reports*, **2016**, 6, 23547	4.9	67
71	Restoring a nearly free-standing character of graphene on Ru(0001) by oxygen intercalation. *Scientific Reports*, **2016**, 6, 20285	4.9	39
70	Post-Hartree-Fock studies of the He/Mg(0001) interaction: Anti-corrugation, screening, and pairwise additivity. *Journal of Chemical Physics*, **2016**, 144, 244707	3.9	13
69	Graphene growth and properties on metal substrates. *Journal of Physics Condensed Matter*, **2015**, 27, 303002	1.8	69
68	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	3.8	30
67	Scanning probe microscopy and spectroscopy of graphene on metals. *Physica Status Solidi (B): Basic Research*, **2015**, 252, 451-468	1.3	23
66	Understanding the origin of band gap formation in graphene on metals: graphene on Cu/Ir(111). *Scientific Reports*, **2014**, 4, 5704	4.9	67
65	Impact of the metal substrate on the electronic structure of armchair graphene nanoribbons. *Chemical Physics Letters*, **2014**, 597, 148-152	2.5	2
64	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	1	2
63	In situ fabrication of quasi-free-standing epitaxial graphene nanoflakes on gold. *ACS Nano*, **2014**, 8, 3735-42	13.7	47
62	Multichannel scanning probe microscopy and spectroscopy of graphene moir structures. *Physical Chemistry Chemical Physics*, **2014**, 16, 3894-908	3.6	23
61	First Multireference Correlation Treatment of Bulk Metals. *Journal of Chemical Theory and Computation*, **2014**, 10, 1698-706	6.4	28
60	Ab initio investigation of ground-state properties of group-12 fluorides. *International Journal of Quantum Chemistry*, **2014**, 114, 943-951	2.1	8
59	Graphene on Rh(111): Combined DFT, STM, and NC-AFM Studies. *Procedia Engineering*, **2014**, 93, 8-16		7
58	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. *Journal of Chemical Physics*, **2014**, 141, 151102	3.9	30
57	Dual character of excited charge carriers in graphene on Ni(111). *Physical Review B*, **2014**, 89,	3.3	7

56	Adsorption of multivalent alkylthiols on Au(111) surface: insights from DFT. *Journal of Computational Chemistry*, **2014**, 35, 204-13	3.5	12
55	General approach to understanding the electronic structure of graphene on metals. *Materials Research Express*, **2014**, 1, 035603	1.7	36
54	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	1.4	5
53	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	3.8	36
52	Structural and electronic properties of graphene-based junctions for spin-filtering: The graphene/Al/Ni(1 1 1) intercalation-like system. *Applied Surface Science*, **2013**, 267, 8-11	6.7	14
51	Specific many-electron effects in X-ray spectra of simple metals and graphene. *Physical Chemistry Chemical Physics*, **2013**, 15, 6749-56	3.6	5
50	Electronic structure and imaging contrast of graphene moir on metals. *Scientific Reports*, **2013**, 3, 1072	4.9	80
49	Theoretical description of X-ray absorption spectroscopy of the graphene-metal interfaces. *Journal of Chemical Physics*, **2013**, 138, 154706	3.9	31
48	Graphene on metallic surfaces: problems and perspectives. *Physical Chemistry Chemical Physics*, **2012**, 14, 13502-14	3.6	144
47	Graphene on Rh(111): Scanning tunneling and atomic force microscopies studies. *Applied Physics Letters*, **2012**, 100, 241606	3.4	88
46	Local correlation method for metals: Benchmarks for surface and adsorption energies. *Physical Review B*, **2012**, 85,	3.3	20
45	Structural and electronic properties of the graphene/Al/Ni(111) intercalation system. *New Journal of Physics*, **2011**, 13, 113028	2.9	95
44	On the physisorption of water on graphene: a CCSD(T) study. *Physical Chemistry Chemical Physics*, **2011**, 13, 12041-7	3.6	152
43	Electronic and Magnetic Properties of the Graphene- Ferromagnet Interfaces: Theory vs. Experiment **2011**,		2
42	Structural and electronic properties of Fe3O4/graphene/Ni(111) junctions. *Physica Status Solidi - Rapid Research Letters*, **2011**, 5, 226-228	2.5	14
41	Graphene on ferromagnetic surfaces and its functionalization with water and ammonia. *Nanoscale Research Letters*, **2011**, 6, 214	5	22
40	Accurate quantum-chemical description of gold complexes with pyridine and its derivatives. *Journal of Computational Chemistry*, **2011**, 32, 1839-45	3.5	15
39	Electronic structure and magnetic properties of the graphene/Fe/Ni111 intercalation-like system. *Physical Chemistry Chemical Physics*, **2011**, 13, 7534-9	3.6	100

38	Theoretical study on the adsorption of pyridine derivatives on graphene. *Chemical Physics Letters*, **2011**, 510, 220-223	2.5	32
37	Development of a Wavefunction-based Ab Initio Method for Metals Applying the Method of Increments. *Zeitschrift Fur Physikalische Chemie*, **2010**, 224, 369-381	3.1	9
36	Preparation and photoemission investigation of bulklike Mn films on W(110). *Physical Review B*, **2010**, 81,	3.3	2
35	The role of electron correlations in the binding properties of Ca, Sr, and Ba. *Journal of Physics Condensed Matter*, **2010**, 22, 275504	1.8	6
34	Induced magnetism of carbon atoms at the graphene/Ni(111) interface. *Applied Physics Letters*, **2010**, 96, 012504	3.4	155
33	Development of a Wavefunction-based Ab Initio Method for Metals Applying the Method of Increments **2010**, 79-91		0
32	First-principles study of the connection between structure and electronic properties of gallium. *Physical Review B*, **2009**, 79,	3.3	26
31	Polarographic and spectrophotometric studies of the spiro[indolin-pyridobenzopyrane] complexes with the heavy metal ions. *Russian Journal of General Chemistry*, **2009**, 79, 1191-1196	0.7	4
30	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	0.7	1
29	Quantum-chemical approach to cohesive properties of metallic beryllium. *Journal of Physics: Conference Series*, **2008**, 117, 012029	0.3	8
28	Spiropyrans and spirooxazines. *Russian Chemical Bulletin*, **2008**, 57, 151-158	1.7	12
27	Cohesive properties of CeN and LaN from first principles. *Journal of Computational Chemistry*, **2008**, 29, 2107-12	3.5	9
26	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	2.8	
25	Correlation energies for small magnesium clusters in comparison with bulk magnesium. *Molecular Physics*, **2007**, 105, 2849-2855	1.7	9
24	Embedding procedure for ab initio correlation calculations in group II metals. *Journal of Chemical Physics*, **2007**, 126, 134115	3.9	40
23	Wave-function-based ab initio method for metals: Application of the incremental scheme to magnesium. *Physical Review B*, **2007**, 75,	3.3	21
22	Observation of surface state on ultrathin fcc Mn(1 1 1) layer. *Surface Science*, **2006**, 600, 4328-4331	1.8	4
21	An attempt to determine the absolute configuration of two ascolactone stereoisomers with time-dependent density functional theory. *Chirality*, **2006**, 18, 413-8	2.1	15

20	Ferromagnetic coupling in EuGd(0001) observed by spin-resolved photoelectron spectroscopy. *Physical Review B*, **2006**, 73,	3.3	5
19	Electronic structure, magnetism, and spin-dependent transport of CeMnNi4. *Physical Review B*, **2006**, 73,	3.3	13
18	Influence of electronic correlations on the ground-state properties of cerium dioxide. *Journal of Chemical Physics*, **2006**, 124, 234711	3.9	30
17	Polyketides from the marine-derived fungus Ascochyta salicorniae and their potential to inhibit protein phosphatases. *Organic and Biomolecular Chemistry*, **2006**, 4, 2233-40	3.9	44
16	First Asymmetric Synthesis and Determination of the Absolute Configuration of a Lignan Isolated from Virola sebifera. *European Journal of Organic Chemistry*, **2005**, 2005, 1984-1990	3.2	11
15	Conformational Analysis and CD Calculations of Methyl-Substituted 13-Tridecano-13-lactones. *Helvetica Chimica Acta*, **2005**, 88, 194-209	2	11
14	On the application of the incremental scheme to ionic solids: test of different embeddings. *Theoretical Chemistry Accounts*, **2005**, 114, 259-264	1.9	10
13	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]. *Russian Chemical Bulletin*, **2005**, 54, 705-710	1.7	8
12	Photochromic properties of six 5-O-n-alkyl,6?-CN substituted spironaphthoxazines. *International Journal of Photoenergy*, **2004**, 6, 199-204	2.1	9
11	Determination of the absolute configuration of calliactine by quantum chemical calculations. *International Journal of Quantum Chemistry*, **2004**, 100, 1104-1113	2.1	10
10	(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	1.4	3
9	Spiropyrans and spirooxazines. 1. Synthesis and photochromic properties of 9"-hydroxy- and 9"-alkoxy-substituted spironaphthooxazines. *Russian Chemical Bulletin*, **2003**, 52, 1172-1181	1.7	16
8	Spiropyrans and spirooxazines. 2. Synthesis, structures, and photochromic properties of 6"-cyano-substituted spironaphthooxazines. *Russian Chemical Bulletin*, **2003**, 52, 2038-2047	1.7	10
7	To Estimation of pKa for Spiropyrans of the Indoline Series. *Russian Journal of General Chemistry*, **2002**, 72, 1468-1472	0.7	4
6	Kinetic and Thermodynamic Investigations of the Photochromism and Solvatochromism of Semipermanent Merocyanines. *Journal of Physical Chemistry A*, **2001**, 105, 8417-8422	2.8	48
5	Photochromism of Spirooxazines in Homogeneous Solution and Phospholipid Liposomes. *Journal of the American Chemical Society*, **1998**, 120, 12707-12713	16.4	94
4	New formyl-substituted spiropyrans of the indoline series. *Chemistry of Heterocyclic Compounds*, **1997**, 32, 1427-1428	1.4	
3	Wavefunction-based ab initio correlation method for metals: application of the incremental scheme to Be, Mg, Zn, Cd, and Hg. *Chemical Modelling*,162-209	2	3

2	Modification of the Magnetic and Electronic Properties of the Graphene-Ni(111) Interface via Halogens Intercalation. *Advanced Theory and Simulations*,2100319	3.5	1
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	