Elena Bichoutskaia

List of Publications by Year
in descending order

135	4,726	134610	124990
papers	citations	34 h-index	64 g-index

140	140	140	7435
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Designing stable binary endohedral fullerene lattices. Physical Chemistry Chemical Physics, 2022, 24, 10044-10052.	1.3	2
2	Computational Predictions for Effective Separation of Xenon/Krypton Gas Mixtures in the MFM Family of Metalâ€“Organic Frameworks. Journal of Physical Chemistry C, 2022, 126, 11475-11486.	1.5	7
3	A high-throughput screening of metalâ€“organic framework based membranes for biogas upgrading. Faraday Discussions, 2021, 231, 235-257.	1.6	12
4	Selective Gas Uptake and Rotational Dynamics in a (3,24)-Connected Metalâ€“Organic Framework Material. Journal of the American Chemical Society, 2021, 143, 3348-3358.	6.6	39
5	N-doping enabled defect-engineering of MoS2 for enhanced and selective adsorption of CO2: A DFT approach. Applied Surface Science, 2021, 542, 148556.	3.1	37
6	The influence of surface charge on the coalescence of ice and dust particles in the mesosphere and lower thermosphere. Atmospheric Chemistry and Physics, 2021, 21, 8735-8745.	1.9	4
7	Fission gas released from molten salt reactor fuel: the case of noble gas short life radioisotopes for radiopharmaceutical application. Medicine in Novel Technology and Devices, 2021, 10, 100057.	0.9	4
8	Triplet Excitation and Electroluminescence from a Supramolecular Monolayer Embedded in a Boron Nitride Tunnel Barrier. Nano Letters, 2020, 20, 278-283.	4.5	9
9	Porous Metalâ€“Organic Polyhedra: Morphology, Porosity, and Guest Binding. Inorganic Chemistry, 2020, 59, 15646-15658.	1.9	16
10	Molecular Quantum Rings Formed from a <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:mi>Ï€</mml:mi></mml:mrow></mml:math> -Conjugated Macrocycle. Physical Review Letters, 2020, 125, 206803.	2.9	19
11	Noncovalent passivation of supported phosphorene for device applications: from morphology to electronic properties. Physical Chemistry Chemical Physics, 2020, 22, 12482-12488.	1.3	6
12	Bond Dissociation and Reactivity of HF and H₂O in a Nano Test Tube. ACS Nano, 2020, 14, 11178-11189.	7.3	17
13	Atomic mechanism of metal crystal nucleus formation in a single-walled carbon nanotube. Nature Chemistry, 2020, 12, 921-928.	6.6	58
14	Low dimensional nanostructures of fast ion conducting lithium nitride. Nature Communications, 2020, 11, 4492.	5.8	19
15	Probing Chemical Kinetics in Two Dimensional Materials Using Atomic Resolution Imaging.. Microscopy and Microanalysis, 2020, 26, 90-90.	0.2	0
16	The Interaction of Hydrogen with the van der Waals Crystal Î³-InSe. Molecules, 2020, 25, 2526.	1.7	11
17	Selfâ€Assembly Behavior of Oppositely Charged Inverse Bipatchy Microcolloids. Small, 2020, 16, e2000442.	5.2	9
18	Imaging an unsupported metalâ€“metal bond in dirhenium molecules at the atomic scale. Science Advances, 2020, 6, eaay5849.	4.7	30

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19	Electrostatic interactions between spheroidal dielectric particles. Journal of Chemical Physics, 2020, 152, 024121.	1.2	14
20	Epitaxial multilayers of alkanes on two-dimensional black phosphorus as passivating and electrically insulating nanostructures. Nanoscale, 2019, 11, 17252-17261.	2.8	13
21	Ordering, flexibility and frustration in arrays of porphyrin nanorings. Nature Communications, 2019, 10, 2932.	5.8	16
22	Interaction between particles with inhomogeneous surface charge distributions: Revisiting the Coulomb fission of dication molecular clusters. Journal of Chemical Physics, 2019, 151, 154113.	1.2	4
23	Observing Structural Dynamics and Measuring Chemical Kinetics in Low Dimensional Materials Using High Speed Imaging. Microscopy and Microanalysis, 2019, 25, 1682-1683.	0.2	2
24	Resonant inelastic X-ray scattering of a Ru photosensitizer: Insights from individual ligands to the electronic structure of the complete molecule. Journal of Chemical Physics, 2019, 151, 074701.	1.2	12
25	The effects of encapsulation on damage to molecules by electron radiation. Micron, 2019, 120, 96-103.	1.1	14
26	Steric and Electronic Control of 1,3-Dipolar Cycloaddition Reactions in Carbon Nanotube Nanoreactors. Journal of Physical Chemistry C, 2019, 123, 6294-6302.	1.5	13
27	Synthesis and characterisation of rylene diimide dimers using molecular handcuffs. Chemical Science, 2019, 10, 3723-3732.	3.7	28
28	Enhancement of CO₂ Uptake and Selectivity in a Metalâ€“Organic Framework by the Incorporation of Thiophene Functionality. Inorganic Chemistry, 2018, 57, 5074-5082.	1.9	50
29	Dynamic simulations of many-body electrostatic self-assembly. Philosophical Transactions Series A, Mathematical, Physical, and Engineering Sciences, 2018, 376, 20170143.	1.6	11
30	Electrostatic Self-Assembly: Understanding the Significance of the Solvent. Journal of Chemical Theory and Computation, 2018, 14, 905-915.	2.3	31
31	Implanting Germanium into Graphene. ACS Nano, 2018, 12, 4641-4647.	7.3	86
32	Adsorption of Hexacontane on Hexagonal Boron Nitride. Journal of Physical Chemistry C, 2018, 122, 27575-27581.	1.5	9
33	Atomistic Simulations of the Efficiencies of Ge and Pt Ion Implantation into Graphene. Journal of Physical Chemistry C, 2018, 122, 25700-25708.	1.5	6
34	The growth and fluorescence of phthalocyanine monolayers, thin films and multilayers on hexagonal boron nitride. Chemical Communications, 2018, 54, 12021-12024.	2.2	12
35	Pore-filling contamination in metalâ€“organic frameworks. Physical Chemistry Chemical Physics, 2018, 20, 23616-23624.	1.3	4
36	Comparison of atomic scale dynamics for the middle and late transition metal nanocatalysts. Nature Communications, 2018, 9, 3382.	5.8	35

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37	Substrate-induced shifts and screening in the fluorescence spectra of supramolecular adsorbed organic monolayers. Journal of Chemical Physics, 2018, 149, 054701.	1.2	22
38	An integral equation approach to calculate electrostatic interactions in many-body dielectric systems. Journal of Computational Physics, 2018, 371, 712-731.	1.9	28
39	Electrostatic interactions between charged dielectric particles in an electrolyte solution: constant potential boundary conditions. Soft Matter, 2018, 14, 5480-5487.	1.2	16
40	The effect of like-charge attraction on aerosol growth in the atmosphere of Titan. Icarus, 2017, 291, 245-253.	1.1	18
41	Stop-Frame Filming and Discovery of Reactions at the Single-Molecule Level by Transmission Electron Microscopy. ACS Nano, 2017, 11, 2509-2520.	7.3	46
42	Tailoring porosity and rotational dynamics in a series of octacarboxylate metal-organic frameworks. Proceedings of the National Academy of Sciences of the United States of America, 2017, 114, 3056-3061.	3.3	73
43	Coulomb fission in multiply charged molecular clusters: Experiment and theory. Journal of Chemical Physics, 2017, 146, 164302.	1.2	6
44	The right isotherms for the right reasons? Validation of generic force fields for prediction of methane adsorption in metal-organic frameworks. Molecular Simulation, 2017, 43, 828-837.	0.9	18
45	Supramolecular heterostructures formed by sequential epitaxial deposition of two-dimensional hydrogen-bonded arrays. Nature Chemistry, 2017, 9, 1191-1197.	6.6	79
46	Chemical Reactions of Molecules Promoted and Simultaneously Imaged by the Electron Beam in Transmission Electron Microscopy. Accounts of Chemical Research, 2017, 50, 1797-1807.	7.6	79
47	Investigation of the Interactions and Bonding between Carbon and Group VIII Metals at the Atomic Scale. Small, 2016, 12, 1649-1657.	5.2	27
48	Computational Evaluation of the Impact of Incorporated Nitrogen and Oxygen Heteroatoms on the Affinity of Polyaromatic Ligands for Carbon Dioxide and Methane in Metalâ€“Organic Frameworks. Journal of Physical Chemistry C, 2016, 120, 27342-27348.	1.5	9
49	Electrostatic interactions between charged dielectric particles in an electrolyte solution. Journal of Chemical Physics, 2016, 145, 084103.	1.2	30
50	Reaction kinetics of bond rotations in graphene. Carbon, 2016, 105, 176-182.	5.4	18
51	Effective Binding of Methane Using a Weak Hydrogen Bond. Journal of Physical Chemistry A, 2016, 120, 3701-3709.	1.1	7
52	Dynamic Behavior of Single Fe Atoms Embedded in Graphene. Journal of Physical Chemistry C, 2016, 120, 21998-22003.	1.5	25
53	Amides Do Not Always Work: Observation of Guest Binding in an Amide-Functionalized Porous Metalâ€“Organic Framework. Journal of the American Chemical Society, 2016, 138, 14828-14831.	6.6	44
54	Direct Measurement of Electron Transfer in Nanoscale Hostâ€“Guest Systems: Metallocenes in Carbon Nanotubes. Chemistry - A European Journal, 2016, 22, 13540-13549.	1.7	18

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55	The influence hydrogen atom addition has on charge switching during motion of the metal atom in endohedral Ca@C ₆₀ H ₄ isomers. Philosophical Transactions Series A, Mathematical, Physical, and Engineering Sciences, 2016, 374, 20150319.	1.6	3
56	Growth of single-layer boron nitride dome-shaped nanostructures catalysed by iron clusters. Nanoscale, 2016, 8, 15079-15085.	2.8	5
57	Observation of Binding and Rotation of Methane and Hydrogen within a Functional Metalâ€“Organic Framework. Journal of the American Chemical Society, 2016, 138, 9119-9127.	6.6	54
58	Stabilising the lowest energy charge-separated state in a {metal chromophore â€“ fullerene} assembly: a tuneable panchromatic absorbing donorâ€“acceptor triad. Chemical Science, 2016, 7, 5908-5921.	3.7	15
59	Mechanisms of monovacancy diffusion in graphene. Chemical Physics Letters, 2016, 648, 161-165.	1.2	24
60	Progress in the theory of electrostatic interactions between charged particles. Physical Chemistry Chemical Physics, 2016, 18, 5883-5895.	1.3	42
61	Electron beam controlled covalent attachment of small organic molecules to graphene. Nanoscale, 2016, 8, 2711-2719.	2.8	28
62	Epitaxial Retrieval of a Disappearing Polymorph. Crystal Growth and Design, 2015, 15, 115-123.	1.4	10
63	Transmission Electron Microscopy: Isotope Substitution Extends the Lifetime of Organic Molecules in Transmission Electron Microscopy (Small 5/2015). Small, 2015, 11, 510-510.	5.2	4
64	A General Geometric Representation of Sphere-Sphere Interactions. Progress in Theoretical Chemistry and Physics, 2015, , 29-36.	0.2	3
65	Energetics of atomic scale structure changes in graphene. Chemical Society Reviews, 2015, 44, 3143-3176.	18.7	141
66	Adsorbate-Induced Curvature and Stiffening of Graphene. Nano Letters, 2015, 15, 159-164.	4.5	24
67	Switching intermolecular interactions by confinement in carbon nanotubes. Chemical Communications, 2015, 51, 648-651.	2.2	5
68	Isotope Substitution Extends the Lifetime of Organic Molecules in Transmission Electron Microscopy. Small, 2015, 11, 622-629.	5.2	39
69	Cyclometallated platinum(<scp>ii</scp>) complexes containing NHC ligands: synthesis, characterization, photophysics and their application as emitters in OLEDs. Dalton Transactions, 2015, 44, 7152-7162.	1.6	37
70	Band gap expansion, shear inversion phase change behaviour and low-voltage induced crystal oscillation in low-dimensional tin selenide crystals. Dalton Transactions, 2014, 43, 7391-7399.	1.6	26
71	Electrostatic force between a charged sphere and a planar surface: A general solution for dielectric materials. Journal of Chemical Physics, 2014, 140, 074107.	1.2	46
72	A Novel Bismuthâ€Based Metalâ€“Organic Framework for High Volumetric Methane and Carbon Dioxide Adsorption. Chemistry - A European Journal, 2014, 20, 8024-8029.	1.7	67

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73	Formation of nickelâ€“carbon heterofullerenes under electron irradiation. Dalton Transactions, 2014, 43, 7499-7513.	1.6	12
74	Polarisation charge switching through the motion of metal atoms trapped in fullerene cages. Physical Chemistry Chemical Physics, 2014, 16, 23869-23873.	1.3	12
75	Analysis of High and Selective Uptake of CO₂ in an Oxamideâ€Containing {Cu₂(OOCR)₄}â€Based Metalâ€“Organic Framework. Chemistry - A European Journal, 2014, 20, 7317-7324.	1.7	119
76	A Robust Binary Supramolecular Organic Framework (SOF) with High CO₂ Adsorption and Selectivity. Journal of the American Chemical Society, 2014, 136, 12828-12831.	6.6	287
77	Methane Adsorption in Metalâ€“Organic Frameworks Containing Nanographene Linkers: A Computational Study. Journal of Physical Chemistry C, 2014, 118, 15573-15580.	1.5	17
78	Transition Metal Complexes of a Salenâ€“Fullerene Diad: Redox and Catalytically Active Nanostructures for Delivery of Metals in Nanotubes. Chemistry - A European Journal, 2013, 19, 11999-12008.	1.7	15
79	Approaches to modelling irradiation-induced processes in transmission electron microscopy. Nanoscale, 2013, 5, 6677.	2.8	32
80	Modulating the packing of [Cu24(isophthalate)24] cuboctahedra in a triazole-containing metalâ€“organic polyhedral framework. Chemical Science, 2013, 4, 1731.	3.7	123
81	Electron-beam engineering of single-walled carbon nanotubes from bilayer graphene. Carbon, 2013, 65, 80-86.	5.4	26
82	Surface-charge distribution on a dielectric sphere due to an external point charge: examples of C60 and C240 fullerenes. Physical Chemistry Chemical Physics, 2013, 15, 20115.	1.3	9
83	Stability and dynamics of vacancy in graphene flakes: Edge effects. Chemical Physics Letters, 2013, 557, 80-87.	1.2	35
84	Inclusion of radiation damage dynamics in high-resolution transmission electron microscopy image simulations: The example of graphene. Physical Review B, 2013, 87, .	1.1	31
85	Meso-scale modelling of shock wave propagation in a SiC/Al nanocomposite reinforced with WS2-inorganic fullerene nanoparticles. Composite Structures, 2013, 96, 601-605.	3.1	9
86	Coulomb Fission in Dielectric Dication Clusters: Experiment and Theory on Steps That May Underpin the Electrospray Mechanism. Journal of Physical Chemistry A, 2013, 117, 3877-3886.	1.1	12
87	Electronic excitation in bulk and nanocrystalline alkali halides. Journal of Chemical Physics, 2012, 137, 184104.	1.2	3
88	Interactions and Reactions of Transition Metal Clusters with the Interior of Single-Walled Carbon Nanotubes Imaged at the Atomic Scale. Journal of the American Chemical Society, 2012, 134, 3073-3079.	6.6	83
89	Reply to the â€˜Comment on â€œTreating highly charged carbon and fullerene clusters as dielectric particlesâ€â€™ by H. Zettergren and H. Cederquist, Phys. Chem. Chem. Phys., 2012, 14, DOI: 10.1039/c2cp42883k Physical Chemistry Chemical Physics, 2012, 14, 16771.	1.3	4
90	Aberration corrected imaging of a carbon nanotube encapsulated Lindqvist Ion and correlation with Density Functional Theory. Journal of Physics: Conference Series, 2012, 371, 012018.	0.3	1

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91	Controlling the Regioselectivity of the Hydrosilylation Reaction in Carbon Nanoreactors. Chemistry - A European Journal, 2012, 18, 13180-13187.	1.7	47
92	Size, Structure, and Helical Twist of Graphene Nanoribbons Controlled by Confinement in Carbon Nanotubes. ACS Nano, 2012, 6, 3943-3953.	7.3	134
93	Sequential multiscale modelling of SiC/Al nanocomposites reinforced with WS<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mrow /><mml:mn>2</mml:mn></mml:msub></mml:math>nanoparticles under static loading. Physical Review B, 2012, 86, .	1.1	6
94	Absolute electrostatic force between two charged particles in a low dielectric solvent. Soft Matter, 2012, 8, 6210.	1.2	13
95	Selective CO2 uptake and inverse CO2/C2H2 selectivity in a dynamic bifunctional metalâ€“organic framework. Chemical Science, 2012, 3, 2993.	3.7	117
96	A partially interpenetrated metalâ€“organic framework for selective hysteretic sorption ofÂcarbon dioxide. Nature Materials, 2012, 11, 710-716.	13.3	430
97	High-precision imaging of an encapsulated Lindqvist ion and correlation of its structure and symmetry with quantum chemical calculations. Nanoscale, 2012, 4, 1190.	2.8	11
98	Treating highly charged carbon and fullerene clusters as dielectric particles. Physical Chemistry Chemical Physics, 2011, 13, 18339-18346.	1.3	18
99	Self-assembly of a sulphur-terminated graphene nanoribbon within a single-walled carbon nanotube. Nature Materials, 2011, 10, 687-692.	13.3	253
100	Reactions of the inner surface of carbon nanotubes and nanoprotrusion processes imaged at the atomic scale. Nature Chemistry, 2011, 3, 732-737.	6.6	83
101	Why like-charged particles of dielectric materials can be attracted to one another. Journal of Colloid and Interface Science, 2011, 354, 417-420.	5.0	35
102	Chapter 8. Theoretical Strategies for Functionalisation and Encapsulation of Nanotubes. RSC Theoretical and Computational Chemistry Series, 2011, , 225-278.	0.7	0
103	High Frequency Electromechanical Memory Cells Based on Telescoping Carbon Nanotubes. Journal of Nanoscience and Nanotechnology, 2010, 10, 4322-4328.	0.9	1
104	Direct transformation of graphene to fullerene. Nature Chemistry, 2010, 2, 450-453.	6.6	361
105	Electrostatic analysis of the interactions between charged particles of dielectric materials. Journal of Chemical Physics, 2010, 133, 024105.	1.2	95
106	Study of polycyclic aromatic hydrocarbons adsorbed on graphene using density functional theory with empirical dispersion correction. Physical Chemistry Chemical Physics, 2010, 12, 6483.	1.3	85
107	Nanoresonator Based on Relative Vibrations of the Walls of Carbon Nanotubes. Fullerenes Nanotubes and Carbon Nanostructures, 2010, 18, 523-530.	1.0	9
108	Modeling of an ultrahigh-frequency resonator based on the relative vibrations of carbon nanotubes. Physical Review B, 2009, 80, .	1.1	24

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109	Ab initio calculations of the walls shear strength of carbon nanotubes. Technical Physics Letters, 2009, 35, 666-669.	0.2	12
110	An electromechanical nanothermometer based on thermal vibrations of carbon nanotube walls. Physics of the Solid State, 2009, 51, 1306-1314.	0.2	6
111	Nanotube-based data storage devices. Materials Today, 2008, 11, 38-43.	8.3	30
112	Electromechanical Nanothermometer Based on Carbon Nanotubes. Fullerenes Nanotubes and Carbon Nanostructures, 2008, 16, 352-356.	1.0	2
113	A theoretical study of the cohesion of noble gases on graphite. Journal of Chemical Physics, 2008, 128, 024709.	1.2	20
114	Theoretical study of the structures and electronic properties of all-surface KI and CsI nanocrystals encapsulated in single walled carbon nanotubes. Journal of Chemical Physics, 2008, 129, 154701.	1.2	13
115	Nanorelay Based on Multiâ€walled Nanotubes. Fullerenes Nanotubes and Carbon Nanostructures, 2008, 16, 340-343.	1.0	3
116	Modelling interwall interactions in carbon nanotubes: fundamentals and device applications. Philosophical Transactions Series A, Mathematical, Physical, and Engineering Sciences, 2007, 365, 2893-2906.	1.6	6
117	Polarizability of the Iodide Ion in Crystal. Journal of Physical Chemistry C, 2007, 111, 9548-9561.	1.5	11
118	Electromechanical nanothermometer. Physics Letters, Section A: General, Atomic and Solid State Physics, 2007, 366, 480-486.	0.9	23
119	Nanoelectromechanical systems based on multi-walled nanotubes: nanothermometer, nanorelay, and nanoactuator. Physica Status Solidi (A) Applications and Materials Science, 2007, 204, 1911-1917.	0.8	39
120	Diffusion of Walls in Doubleâ€Walled Carbon Nanotubes. Fullerenes Nanotubes and Carbon Nanostructures, 2006, 14, 215-220.	1.0	5
121	Interwall interaction and elastic properties of carbon nanotubes. Physical Review B, 2006, 73, .	1.1	59
122	Fundamental Global Model for the Structures and Energetics of Nanocrystalline Ionic Solids. Journal of Physical Chemistry B, 2006, 110, 5936-5949.	1.2	13
123	Multiâ€Walled Nanotubes: Commensurateâ€Incommensurate Phase Transition and NEMS Applications. Fullerenes Nanotubes and Carbon Nanostructures, 2006, 14, 131-140.	1.0	25
124	Structure and energetics of LiF chains as a model for low dimensional alkali halide nanocrystals. Chemical Physics Letters, 2006, 423, 234-239.	1.2	7
125	Ab initiostudy of relative motion of walls in carbon nanotubes. Physical Review B, 2005, 71, .	1.1	48
126	Extrapolation methods and scaled perturbation theory for determining intermolecular potential energy surfaces. International Journal of Quantum Chemistry, 2004, 96, 537-546.	1.0	5

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127	Ab initio spectroscopy of Van der Waals molecules: a comparison of three different theoretical methods applied to NeHF and NeDF. Chemical Physics Letters, 2004, 393, 70-75.	1.2	1
128	Intermolecular potential energy extrapolation method for weakly bound systems: Ar2, Arâ€“H2and Arâ€“HF dimers. Molecular Physics, 2004, 102, 567-577.	0.8	8
129	Intermolecular potentials from supermolecule and monomer calculations. International Reviews in Physical Chemistry, 2004, 23, 151-185.	0.9	22
130	Perturbative, acausal effects in ultracold non-crossing atomic collisions. Journal of Physics B: Atomic, Molecular and Optical Physics, 2003, 36, 11-18.	0.6	1
131	On the semiclassical approach to cold atomic collisions. Proceedings of the Royal Society A: Mathematical, Physical and Engineering Sciences, 2002, 458, 1399-1409.	1.0	1
132	Semiclassical analytical approach to the description of quasimolecular optical transitions. Journal of Physics B: Atomic, Molecular and Optical Physics, 2002, 35, 2469-2475.	0.6	5
133	Extrapolation of intermolecular interaction energies in weakly bound Van der Waals complexes. Journal of Computational Methods in Sciences and Engineering, 2002, 2, 391-397.	0.1	6
134	Spectroscopy of quasimolecular optical transitions: Ca(4s21S0â†”4s4p1P,4s3d1D2)-He. The influence of radiation width. Journal of Physics B: Atomic, Molecular and Optical Physics, 2001, 34, 2301-2312.	0.6	7
135	Quasi-molecular emission and nonadiabatic transitions: II. Ca(4s4p 1 P, 4s3d 1 D)-He(1s 2, 1 S 0) quasi-molecule. Optics and Spectroscopy (English Translation of Optika I Spektroskopiya), 2000, 88, 163-168.	0.2	1