Elena Bichoutskaia

List of Publications by Year in Descending Order

134 papers	3,748 citations	30 h-index	57 g-index
140 ext. papers	4,255 ext. citations	6.8 avg, IF	5.3 L-index

#	Paper	IF	Citations
134	N-doping enabled defect-engineering of MoS2 for enhanced and selective adsorption of CO2: A DFT approach. *Applied Surface Science*, **2021**, 542, 148556	6.7	14
133	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	6.8	1
132	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	2.1	0
131	A high-throughput screening of metal-organic framework based membranes for biogas upgrading. *Faraday Discussions*, **2021**, 231, 235-257	3.6	2
130	Selective Gas Uptake and Rotational Dynamics in a (3,24)-Connected Metal-Organic Framework Material. *Journal of the American Chemical Society*, **2021**, 143, 3348-3358	16.4	19
129	The Interaction of Hydrogen with the van der Waals Crystal -InSe. *Molecules*, **2020**, 25,	4.8	8
128	Self-Assembly Behavior of Oppositely Charged Inverse Bipatchy Microcolloids. *Small*, **2020**, 16, e2000442	11	5
127	Imaging an unsupported metal-metal bond in dirhenium molecules at the atomic scale. *Science Advances*, **2020**, 6, eaay5849	14.3	15
126	Electrostatic interactions between spheroidal dielectric particles. *Journal of Chemical Physics*, **2020**, 152, 024121	3.9	6
125	Triplet Excitation and Electroluminescence from a Supramolecular Monolayer Embedded in a Boron Nitride Tunnel Barrier. *Nano Letters*, **2020**, 20, 278-283	11.5	5
124	Porous Metal-Organic Polyhedra: Morphology, Porosity, and Guest Binding. *Inorganic Chemistry*, **2020**, 59, 15646-15658	5.1	6
123	Molecular Quantum Rings Formed from a Conjugated Macrocycle. *Physical Review Letters*, **2020**, 125, 206803	7.4	7
122	Noncovalent passivation of supported phosphorene for device applications: from morphology to electronic properties. *Physical Chemistry Chemical Physics*, **2020**, 22, 12482-12488	3.6	4
121	Bond Dissociation and Reactivity of HF and HO in a Nano Test Tube. *ACS Nano*, **2020**, 14, 11178-11189	16.7	7
120	Atomic mechanism of metal crystal nucleus formation in a single-walled carbon nanotube. *Nature Chemistry*, **2020**, 12, 921-928	17.6	25
119	Low dimensional nanostructures of fast ion conducting lithium nitride. *Nature Communications*, **2020**, 11, 4492	17.4	6
118	Probing Chemical Kinetics in Two Dimensional Materials Using Atomic Resolution Imaging.. *Microscopy and Microanalysis*, **2020**, 26, 90-90	0.5	

117	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	3.9	8
116	The effects of encapsulation on damage to molecules by electron radiation. *Micron*, **2019**, 120, 96-103	2.3	8
115	Steric and Electronic Control of 1,3-Dipolar Cycloaddition Reactions in Carbon Nanotube Nanoreactors. *Journal of Physical Chemistry C*, **2019**, 123, 6294-6302	3.8	6
114	Epitaxial multilayers of alkanes on two-dimensional black phosphorus as passivating and electrically insulating nanostructures. *Nanoscale*, **2019**, 11, 17252-17261	7.7	11
113	Ordering, flexibility and frustration in arrays of porphyrin nanorings. *Nature Communications*, **2019**, 10, 2932	17.4	10
112	Interaction between particles with inhomogeneous surface charge distributions: Revisiting the Coulomb fission of dication molecular clusters. *Journal of Chemical Physics*, **2019**, 151, 154113	3.9	1
111	Observing Structural Dynamics and Measuring Chemical Kinetics in Low Dimensional Materials Using High Speed Imaging. *Microscopy and Microanalysis*, **2019**, 25, 1682-1683	0.5	1
110	Synthesis and characterisation of rylene diimide dimers using molecular handcuffs. *Chemical Science*, **2019**, 10, 3723-3732	9.4	20
109	Enhancement of CO Uptake and Selectivity in a Metal-Organic Framework by the Incorporation of Thiophene Functionality. *Inorganic Chemistry*, **2018**, 57, 5074-5082	5.1	26
108	Dynamic simulations of many-body electrostatic self-assembly. *Philosophical Transactions Series A, Mathematical, Physical, and Engineering Sciences*, **2018**, 376,	3	6
107	Electrostatic Self-Assembly: Understanding the Significance of the Solvent. *Journal of Chemical Theory and Computation*, **2018**, 14, 905-915	6.4	17
106	Implanting Germanium into Graphene. *ACS Nano*, **2018**, 12, 4641-4647	16.7	56
105	Comparison of atomic scale dynamics for the middle and late transition metal nanocatalysts. *Nature Communications*, **2018**, 9, 3382	17.4	20
104	Substrate-induced shifts and screening in the fluorescence spectra of supramolecular adsorbed organic monolayers. *Journal of Chemical Physics*, **2018**, 149, 054701	3.9	16
103	An integral equation approach to calculate electrostatic interactions in many-body dielectric systems. *Journal of Computational Physics*, **2018**, 371, 712-731	4.1	14
102	Electrostatic interactions between charged dielectric particles in an electrolyte solution: constant potential boundary conditions. *Soft Matter*, **2018**, 14, 5480-5487	3.6	9
101	Adsorption of Hexacontane on Hexagonal Boron Nitride. *Journal of Physical Chemistry C*, **2018**, 122, 27575-27581	3.8	4
100	Atomistic Simulations of the Efficiencies of Ge and Pt Ion Implantation into Graphene. *Journal of Physical Chemistry C*, **2018**, 122, 25700-25708	3.8	3

99	The growth and fluorescence of phthalocyanine monolayers, thin films and multilayers on hexagonal boron nitride. *Chemical Communications*, **2018**, 54, 12021-12024	5.8	8
98	Pore-filling contamination in metal-organic frameworks. *Physical Chemistry Chemical Physics*, **2018**, 20, 23616-23624	3.6	4
97	The effect of like-charge attraction on aerosol growth in the atmosphere of Titan. *Icarus*, **2017**, 291, 245-253	3.3	13
96	Stop-Frame Filming and Discovery of Reactions at the Single-Molecule Level by Transmission Electron Microscopy. *ACS Nano*, **2017**, 11, 2509-2520	16.7	38
95	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	11.5	57
94	Coulomb fission in multiply charged molecular clusters: Experiment and theory. *Journal of Chemical Physics*, **2017**, 146, 164302	3.9	5
93	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	2	12
92	Supramolecular heterostructures formed by sequential epitaxial deposition of two-dimensional hydrogen-bonded arrays. *Nature Chemistry*, **2017**, 9, 1191-1197	17.6	62
91	Chemical Reactions of Molecules Promoted and Simultaneously Imaged by the Electron Beam in Transmission Electron Microscopy. *Accounts of Chemical Research*, **2017**, 50, 1797-1807	24.3	48
90	The influence hydrogen atom addition has on charge switching during motion of the metal atom in endohedral Ca@C60H4 isomers. *Philosophical Transactions Series A, Mathematical, Physical, and Engineering Sciences*, **2016**, 374,	3	1
89	Growth of single-layer boron nitride dome-shaped nanostructures catalysed by iron clusters. *Nanoscale*, **2016**, 8, 15079-85	7.7	1
88	Observation of Binding and Rotation of Methane and Hydrogen within a Functional Metal-Organic Framework. *Journal of the American Chemical Society*, **2016**, 138, 9119-27	16.4	48
87	Imaging of Electron Beam Triggered Phase Transformations and Chemical Reactions of Organic Molecules by Aberration-Corrected Low-Voltage Transmission Electron Microscopy **2016**, 171-172		
86	Stabilising the lowest energy charge-separated state in a {metal chromophore - fullerene} assembly: a tuneable panchromatic absorbing donor-acceptor triad. *Chemical Science*, **2016**, 7, 5908-5921	9.4	13
85	Mechanisms of monovacancy diffusion in graphene. *Chemical Physics Letters*, **2016**, 648, 161-165	2.5	15
84	Progress in the theory of electrostatic interactions between charged particles. *Physical Chemistry Chemical Physics*, **2016**, 18, 5883-95	3.6	28
83	Electron beam controlled covalent attachment of small organic molecules to graphene. *Nanoscale*, **2016**, 8, 2711-9	7.7	24
82	In-situ TEM growth of single-layer boron nitride dome-shaped nanostructures catalysed by iron clusters **2016**, 155-156		

81	Investigation of the Interactions and Bonding between Carbon and Group VIII Metals at the Atomic Scale. *Small*, **2016**, 12, 1649-57	11	24
80	Computational Evaluation of the Impact of Incorporated Nitrogen and Oxygen Heteroatoms on the Affinity of Polyaromatic Ligands for Carbon Dioxide and Methane in Metal Organic Frameworks. *Journal of Physical Chemistry C*, **2016**, 120, 27342-27348	3.8	6
79	Electrostatic interactions between charged dielectric particles in an electrolyte solution. *Journal of Chemical Physics*, **2016**, 145, 084103	3.9	20
78	Reaction kinetics of bond rotations in graphene. *Carbon*, **2016**, 105, 176-182	10.4	16
77	Effective Binding of Methane Using a Weak Hydrogen Bond. *Journal of Physical Chemistry A*, **2016**, 120, 3701-9	2.8	3
76	Dynamic Behavior of Single Fe Atoms Embedded in Graphene. *Journal of Physical Chemistry C*, **2016**, 120, 21998-22003	3.8	16
75	Amides Do Not Always Work: Observation of Guest Binding in an Amide-Functionalized Porous Metal-Organic Framework. *Journal of the American Chemical Society*, **2016**, 138, 14828-14831	16.4	38
74	Direct Measurement of Electron Transfer in Nanoscale Host-Guest Systems: Metallocenes in Carbon Nanotubes. *Chemistry - A European Journal*, **2016**, 22, 13540-9	4.8	16
73	A General Geometric Representation of Sphere-Sphere Interactions. *Progress in Theoretical Chemistry and Physics*, **2015**, 29-36	0.6	3
72	Energetics of atomic scale structure changes in graphene. *Chemical Society Reviews*, **2015**, 44, 3143-76	58.5	102
71	Adsorbate-induced curvature and stiffening of graphene. *Nano Letters*, **2015**, 15, 159-64	11.5	20
70	Switching intermolecular interactions by confinement in carbon nanotubes. *Chemical Communications*, **2015**, 51, 648-51	5.8	4
69	Isotope substitution extends the lifetime of organic molecules in transmission electron microscopy. *Small*, **2015**, 11, 622-9	11	33
68	Cyclometallated platinum(II) complexes containing NHC ligands: synthesis, characterization, photophysics and their application as emitters in OLEDs. *Dalton Transactions*, **2015**, 44, 7152-62	4.3	32
67	Epitaxial Retrieval of a Disappearing Polymorph. *Crystal Growth and Design*, **2015**, 15, 115-123	3.5	10
66	Transmission Electron Microscopy: Isotope Substitution Extends the Lifetime of Organic Molecules in Transmission Electron Microscopy (Small 5/2015). *Small*, **2015**, 11, 510-510	11	3
65	A novel bismuth-based metal-organic framework for high volumetric methane and carbon dioxide adsorption. *Chemistry - A European Journal*, **2014**, 20, 8024-9	4.8	55
64	Formation of nickel-carbon heterofullerenes under electron irradiation. *Dalton Transactions*, **2014**, 43, 7499-513	4.3	11

63	Polarisation charge switching through the motion of metal atoms trapped in fullerene cages. *Physical Chemistry Chemical Physics*, **2014**, 16, 23869-73	3.6	9
62	Analysis of high and selective uptake of CO2 in an oxamide-containing {Cu2(OOCR)4}-based metal-organic framework. *Chemistry - A European Journal*, **2014**, 20, 7317-24	4.8	105
61	A robust binary supramolecular organic framework (SOF) with high CO2 adsorption and selectivity. *Journal of the American Chemical Society*, **2014**, 136, 12828-31	16.4	220
60	Methane Adsorption in Metal□Organic Frameworks Containing Nanographene Linkers: A Computational Study. *Journal of Physical Chemistry C*, **2014**, 118, 15573-15580	3.8	16
59	Band gap expansion, shear inversion phase change behaviour and low-voltage induced crystal oscillation in low-dimensional tin selenide crystals. *Dalton Transactions*, **2014**, 43, 7391-9	4.3	18
58	Electrostatic force between a charged sphere and a planar surface: a general solution for dielectric materials. *Journal of Chemical Physics*, **2014**, 140, 074107	3.9	30
57	Transition metal complexes of a salen-fullerene diad: redox and catalytically active nanostructures for delivery of metals in nanotubes. *Chemistry - A European Journal*, **2013**, 19, 11999-2008	4.8	15
56	Approaches to modelling irradiation-induced processes in transmission electron microscopy. *Nanoscale*, **2013**, 5, 6677-92	7.7	29
55	Modulating the packing of [Cu24(isophthalate)24] cuboctahedra in a triazole-containing metal□organic polyhedral framework. *Chemical Science*, **2013**, 4, 1731	9.4	117
54	Electron-beam engineering of single-walled carbon nanotubes from bilayer graphene. *Carbon*, **2013**, 65, 80-86	10.4	21
53	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, 20115-9	3.6	6
52	Stability and dynamics of vacancy in graphene flakes: Edge effects. *Chemical Physics Letters*, **2013**, 557, 80-87	2.5	31
51	Inclusion of radiation damage dynamics in high-resolution transmission electron microscopy image simulations: The example of graphene. *Physical Review B*, **2013**, 87,	3.3	26
50	Meso-scale modelling of shock wave propagation in a SiC/Al nanocomposite reinforced with WS2-inorganic fullerene nanoparticles. *Composite Structures*, **2013**, 96, 601-605	5.3	7
49	Coulomb fission in dielectric dication clusters: experiment and theory on steps that may underpin the electrospray mechanism. *Journal of Physical Chemistry A*, **2013**, 117, 3877-86	2.8	11
48	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, 3073-9	16.4	73
47	Reply to the □comment on □reating highly charged carbon and fullerene clusters as dielectric particles□by H. Zettergren and H. Cederquist, Phys. Chem. Chem. Phys., 2012, 14, DOI: 10.1039/c2cp42883k. *Physical Chemistry Chemical Physics*, **2012**, 14, 16771	3.6	4
46	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

45	Controlling the regioselectivity of the hydrosilylation reaction in carbon nanoreactors. *Chemistry - A European Journal*, **2012**, 18, 13180-7	4.8	38
44	Size, structure, and helical twist of graphene nanoribbons controlled by confinement in carbon nanotubes. *ACS Nano*, **2012**, 6, 3943-53	16.7	118
43	Sequential multiscale modelling of SiC/Al nanocomposites reinforced with WS2 nanoparticles under static loading. *Physical Review B*, **2012**, 86,	3.3	4
42	Absolute electrostatic force between two charged particles in a low dielectric solvent. *Soft Matter*, **2012**, 8, 6210	3.6	11
41	Selective CO2 uptake and inverse CO2/C2H2 selectivity in a dynamic bifunctional metal□organic framework. *Chemical Science*, **2012**, 3, 2993	9.4	104
40	A partially interpenetrated metal-organic framework for selective hysteretic sorption of□carbon dioxide. *Nature Materials*, **2012**, 11, 710-6	27	389
39	High-precision imaging of an encapsulated Lindqvist ion and correlation of its structure and symmetry with quantum chemical calculations. *Nanoscale*, **2012**, 4, 1190-9	7.7	10
38	Electronic excitation in bulk and nanocrystalline alkali halides. *Journal of Chemical Physics*, **2012**, 137, 184104	3.9	3
37	Treating highly charged carbon and fullerene clusters as dielectric particles. *Physical Chemistry Chemical Physics*, **2011**, 13, 18339-46	3.6	16
36	Self-assembly of a sulphur-terminated graphene nanoribbon within a single-walled carbon nanotube. *Nature Materials*, **2011**, 10, 687-92	27	225
35	Reactions of the inner surface of carbon nanotubes and nanoprotrusion processes imaged at the atomic scale. *Nature Chemistry*, **2011**, 3, 732-7	17.6	74
34	Why like-charged particles of dielectric materials can be attracted to one another. *Journal of Colloid and Interface Science*, **2011**, 354, 417-20	9.3	30
33	Direct transformation of graphene to fullerene. *Nature Chemistry*, **2010**, 2, 450-3	17.6	297
32	Electrostatic analysis of the interactions between charged particles of dielectric materials. *Journal of Chemical Physics*, **2010**, 133, 024105	3.9	77
31	Study of polycyclic aromatic hydrocarbons adsorbed on graphene using density functional theory with empirical dispersion correction. *Physical Chemistry Chemical Physics*, **2010**, 12, 6483-91	3.6	72
30	Nanoresonator Based on Relative Vibrations of the Walls of Carbon Nanotubes. *Fullerenes Nanotubes and Carbon Nanostructures*, **2010**, 18, 523-530	1.8	8
29	High frequency electromechanical memory cells based on telescoping carbon nanotubes. *Journal of Nanoscience and Nanotechnology*, **2010**, 10, 4322-8	1.3	0
28	Modeling of an ultrahigh-frequency resonator based on the relative vibrations of carbon nanotubes. *Physical Review B*, **2009**, 80,	3.3	22

27	Ab initio calculations of the walls shear strength of carbon nanotubes. *Technical Physics Letters*, **2009**, 35, 666-669	0.7	11
26	An electromechanical nanothermometer based on thermal vibrations of carbon nanotube walls. *Physics of the Solid State*, **2009**, 51, 1306-1314	0.8	3
25	Electromechanical Nanothermometer Based on Carbon Nanotubes. *Fullerenes Nanotubes and Carbon Nanostructures*, **2008**, 16, 352-356	1.8	2
24	A theoretical study of the cohesion of noble gases on graphite. *Journal of Chemical Physics*, **2008**, 128, 024709	3.9	18
23	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	3.9	13
22	Nanorelay Based on Multi-walled Nanotubes. *Fullerenes Nanotubes and Carbon Nanostructures*, **2008**, 16, 340-343	1.8	3
21	Nanotube-based data storage devices. *Materials Today*, **2008**, 11, 38-43	21.8	27
20	Polarizability of the Iodide Ion in Crystal. *Journal of Physical Chemistry C*, **2007**, 111, 9548-9561	3.8	11
19	Electromechanical nanothermometer. *Physics Letters, Section A: General, Atomic and Solid State Physics*, **2007**, 366, 480-486	2.3	23
18	Nanoelectromechanical systems based on multi-walled nanotubes: nanothermometer, nanorelay, and nanoactuator. *Physica Status Solidi (A) Applications and Materials Science*, **2007**, 204, 1911-1917	1.6	34
17	Modelling interwall interactions in carbon nanotubes: fundamentals and device applications. *Philosophical Transactions Series A, Mathematical, Physical, and Engineering Sciences*, **2007**, 365, 2893-906	3	5
16	Diffusion of Walls in Double-Walled Carbon Nanotubes. *Fullerenes Nanotubes and Carbon Nanostructures*, **2006**, 14, 215-220	1.8	5
15	Interwall interaction and elastic properties of carbon nanotubes. *Physical Review B*, **2006**, 73,	3.3	55
14	Fundamental global model for the structures and energetics of nanocrystalline ionic solids. *Journal of Physical Chemistry B*, **2006**, 110, 5936-49	3.4	13
13	Multi-Walled Nanotubes: Commensurate-Incommensurate Phase Transition and NEMS Applications. *Fullerenes Nanotubes and Carbon Nanostructures*, **2006**, 14, 131-140	1.8	24
12	Structure and energetics of LiF chains as a model for low dimensional alkali halide nanocrystals. *Chemical Physics Letters*, **2006**, 423, 234-239	2.5	7
11	Ab initio study of relative motion of walls in carbon nanotubes. *Physical Review B*, **2005**, 71,	3.3	45
10	Extrapolation methods and scaled perturbation theory for determining intermolecular potential energy surfaces. *International Journal of Quantum Chemistry*, **2004**, 96, 537-546	2.1	5

9	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	2.5	1
8	Intermolecular potential energy extrapolation method for weakly bound systems: Ar2, ArH2 and ArHF dimers. *Molecular Physics*, **2004**, 102, 567-577	1.7	8
7	Intermolecular potentials from supermolecule and monomer calculations. *International Reviews in Physical Chemistry*, **2004**, 23, 151-185	7	22
6	Perturbative, acausal effects in ultracold non-crossing atomic collisions. *Journal of Physics B: Atomic, Molecular and Optical Physics*, **2003**, 36, 11-18	1.3	1
5	On the semiclassical approach to cold atomic collisions. *Proceedings of the Royal Society A: Mathematical, Physical and Engineering Sciences*, **2002**, 458, 1399-1409	2.4	1
4	Semiclassical analytical approach to the description of quasimolecular optical transitions. *Journal of Physics B: Atomic, Molecular and Optical Physics*, **2002**, 35, 2469-2475	1.3	5
3	Extrapolation of intermolecular interaction energies in weakly bound Van der Waals complexes. *Journal of Computational Methods in Sciences and Engineering*, **2002**, 2, 391-397	0.3	6
2	Spectroscopy of quasimolecular optical transitions: Ca(4s21S0<-4s4p1P,4s3d1D2)-He. The influence of radiation width. *Journal of Physics B: Atomic, Molecular and Optical Physics*, **2001**, 34, 2301-2312	1.3	7
1	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	0.7	1