Alexander I Boldyrev

List of Publications by Citations

293 papers	18,183 citations	73 h-index	125 g-index
335 ext. papers	19,954 ext. citations	6.9 avg, IF	7 L-index

#	Paper	IF	Citations
293	Developing paradigms of chemical bonding: adaptive natural density partitioning. *Physical Chemistry Chemical Physics*, **2008**, 10, 5207-17	3.6	911
292	Observation of all-metal aromatic molecules. *Science*, **2001**, 291, 859-61	33.3	531
291	All-boron aromatic clusters as potential new inorganic ligands and building blocks in chemistry. *Coordination Chemistry Reviews*, **2006**, 250, 2811-2866	23.2	509
290	All-metal aromaticity and antiaromaticity. *Chemical Reviews*, **2005**, 105, 3716-57	68.1	457
289	A concentric planar doubly □aromatic B□ cluster. *Nature Chemistry*, **2010**, 2, 202-6	17.6	424
288	Hepta- and octacoordinate boron in molecular wheels of eight- and nine-atom boron clusters: observation and confirmation. *Angewandte Chemie - International Edition*, **2003**, 42, 6004-8	16.4	419
287	Understanding boron through size-selected clusters: structure, chemical bonding, and fluxionality. *Accounts of Chemical Research*, **2014**, 47, 1349-58	24.3	382
286	Structure of the Na(x)Cl(x+1) (-) (x=1-4) clusters via ab initio genetic algorithm and photoelectron spectroscopy. *Journal of Chemical Physics*, **2004**, 121, 5709-19	3.9	247
285	First experimental photoelectron spectra of superhalogens and their theoretical interpretations. *Journal of Chemical Physics*, **1999**, 110, 4763-4771	3.9	243
284	All-boron analogues of aromatic hydrocarbons: B17- and B18-. *Journal of Chemical Physics*, **2011**, 134, 224304	3.9	242
283	Tetracoordinated Planar Carbon in the Al4C- Anion. A Combined Photoelectron Spectroscopy and ab Initio Study. *Journal of the American Chemical Society*, **1999**, 121, 6033-6038	16.4	242
282	Two-dimensional Cu2Si monolayer with planar hexacoordinate copper and silicon bonding. *Journal of the American Chemical Society*, **2015**, 137, 2757-62	16.4	237
281	A photoelectron spectroscopic and theoretical study of B16- and B16(2-): an all-boron naphthalene. *Journal of the American Chemical Society*, **2008**, 130, 7244-6	16.4	231
280	All-metal antiaromatic molecule: rectangular Al4(4-) in the Li3Al4(-) anion. *Science*, **2003**, 300, 622-5	33.3	205
279	Revealing intuitively assessable chemical bonding patterns in organic aromatic molecules via adaptive natural density partitioning. *Journal of Organic Chemistry*, **2008**, 73, 9251-8	4.2	203
278	On the aromaticity of square planar Ga4(2-) and In4(2-) in gaseous NaGa4- and NaIn4- clusters. *Journal of the American Chemical Society*, **2001**, 123, 8825-31	16.4	201
277	A stable compound of helium and sodium at high pressure. *Nature Chemistry*, **2017**, 9, 440-445	17.6	199

276	Comprehensive analysis of chemical bonding in boron clusters. *Journal of Computational Chemistry*, **2007**, 28, 251-68	3.5	193
275	Electronic structure and chemical bonding of B5 and B5 by photoelectron spectroscopy and ab initio calculations. *Journal of Chemical Physics*, **2002**, 117, 7917-7924	3.9	193
274	Experimental Observation of Pentaatomic Tetracoordinate Planar Carbon-Containing Molecules. *Journal of the American Chemical Society*, **2000**, 122, 7681-7687	16.4	188
273	Transition-metal-centered monocyclic boron wheel clusters (M Bn): a new class of aromatic borometallic compounds. *Accounts of Chemical Research*, **2013**, 46, 350-8	24.3	184
272	Search for the Lin(0/+1/-1) (n = 5-7) Lowest-Energy Structures Using the ab Initio Gradient Embedded Genetic Algorithm (GEGA). Elucidation of the Chemical Bonding in the Lithium Clusters. *Journal of Chemical Theory and Computation*, **2005**, 1, 566-80	6.4	181
271	Aromaticity and Antiaromaticity in Alkali Metal and Alkaline Earth Metal Small Clusters. *Journal of Physical Chemistry A*, **2003**, 107, 554-560	2.8	178
270	Electronic Structure, Isomerism, and Chemical Bonding in B7- and B7. *Journal of Physical Chemistry A*, **2004**, 108, 3509-3517	2.8	177
269	Structure and Bonding in B6- and B6: Planarity and Antiaromaticity. *Journal of Physical Chemistry A*, **2003**, 107, 1359-1369	2.8	175
268	B22- and B23-: all-boron analogues of anthracene and phenanthrene. *Journal of the American Chemical Society*, **2012**, 134, 18065-73	16.4	172
267	Photoelectron Spectroscopy and ab Initio Study of B3- and B4- Anions and Their Neutrals. *Journal of Physical Chemistry A*, **2003**, 107, 9319-9328	2.8	169
266	Aromaticity and antiaromaticity in transition-metal systems. *Physical Chemistry Chemical Physics*, **2008**, 10, 257-67	3.6	166
265	A new, general strategy for achieving planar tetracoordinate geometries for carbon and other second row periodic elements. *Journal of the Chemical Society Chemical Communications*, **1991**, 1536-1538		164
264	Observation of the highest coordination number in planar species: decacoordinated Ta B10(-) and Nb B10(-) anions. *Angewandte Chemie - International Edition*, **2012**, 51, 2101-5	16.4	160
263	Small Multiply Charged Anions as Building Blocks in Chemistry. *Accounts of Chemical Research*, **1996**, 29, 497-502	24.3	156
262	Contribution of electron correlation to the stability of dipole-bound anionic states. *Physical Review A*, **1996**, 54, 1906-1909	2.6	156
261	Ab initio study of superalkalis. First ionization potentials and thermodynamic stability. *Inorganic Chemistry*, **1992**, 31, 4834-4842	5.1	155
260	Aromatic metal-centered monocyclic boron rings: Co B8- and Ru B9-. *Angewandte Chemie - International Edition*, **2011**, 50, 9334-7	16.4	151
259	Cobalt-centred boron molecular drums with the highest coordination number in the CoB16- cluster. *Nature Communications*, **2015**, 6, 8654	17.4	147

258	MX3(-) superhalogens (M = Be, Mg, Ca; X = Cl, Br): a photoelectron spectroscopic and ab initio theoretical study. *Journal of Physical Chemistry A*, **2005**, 109, 11560-7	2.8	142
257	Sn12(2-): stannaspherene. *Journal of the American Chemical Society*, **2006**, 128, 8390-1	16.4	140
256	Experimental and Theoretical Observations of Aromaticity in Heterocyclic XAl3□(X=Si, Ge, Sn, Pb) Systems. *Angewandte Chemie - International Edition*, **2001**, 40, 1867-1870	16.4	140
255	Carbon avoids hypercoordination in CB6(-), CB6(2-), and C2B5(-) planar carbon-boron clusters. *Journal of the American Chemical Society*, **2008**, 130, 9248-50	16.4	138
254	Molecular wheel B8(2-) as a new inorganic ligand. photoelectron spectroscopy and ab initio characterization of LiB8(-). *Inorganic Chemistry*, **2004**, 43, 3552-4	5.1	135
253	Aromatic Mercury Clusters in Ancient Amalgams Work done at Utah State University is supported by the donors to The Petroleum Research Fund, administered by the American Chemical Society. Work done at Iowa State University is supported by Basic Energy Sciences, the U.S. Department of Energy. Work done at Washington State University is supported by the National Science	16.4	134
252	Tetracoordinated Planar Carbon in Pentaatomic Molecules. *Journal of the American Chemical Society*, **1998**, 120, 7967-7972	16.4	134
251	Deciphering chemical bonding in golden cages. *Journal of Physical Chemistry A*, **2009**, 113, 866-8	2.8	133
250	On the resonance energy in new all-metal aromatic molecules. *Inorganic Chemistry*, **2002**, 41, 532-7	5.1	133
249	Transition-metal-centered nine-membered boron rings: M(c)B9 and M(c)B9(-) (M = Rh, Ir). *Journal of the American Chemical Society*, **2012**, 134, 165-8	16.4	132
248	Theoretical Evidence of Aromaticity in X3 □(X = B, Al, Ga) Species. *Structural Chemistry*, **2002**, 13, 141-148	1.8	123
247	Deciphering the mystery of hexagon holes in an all-boron graphene □sheet. *Physical Chemistry Chemical Physics*, **2011**, 13, 11575-8	3.6	122
246	Al(6)(2-) - fusion of two aromatic Al(3)(-) units. A combined photoelectron spectroscopy and ab initio study of M(+)[Al(6)(2-)] (M = Li, Na, K, Cu, and Au). *Journal of the American Chemical Society*, **2002**, 124, 11791-801	16.4	121
245	The Electronic Structure of Superhalogens and Superalkalies. *Russian Chemical Reviews*, **1987**, 56, 519-536	1.8	119
244	Isolated SO42- and PO43- Anions Do Not Exist. *The Journal of Physical Chemistry*, **1994**, 98, 2298-2300		118
243	Delta aromaticity in [Ta3O3]-. *Angewandte Chemie - International Edition*, **2007**, 46, 4277-80	16.4	115
242	A photoelectron spectroscopy and ab initio study of B21-: negatively charged boron clusters continue to be planar at 21. *Journal of Chemical Physics*, **2012**, 136, 104310	3.9	112
241	Adiabatic electron affinities of small superhalogens: LiF2, LiCl2, NaF2, and NaCl2. *Journal of Chemical Physics*, **1997**, 107, 3867-3875	3.9	112

240	Ab initio study of the electronic structures of lithium containing diatomic molecules and ions. *Journal of Chemical Physics*, **1993**, 99, 8793-8804	3.9	112
239	Complexes between planar boron clusters and transition metals: a photoelectron spectroscopy and ab initio study of CoB12(-) and RhB12(-). *Journal of Physical Chemistry A*, **2014**, 118, 8098-105	2.8	111
238	Solid state adaptive natural density partitioning: a tool for deciphering multi-center bonding in periodic systems. *Physical Chemistry Chemical Physics*, **2013**, 15, 5022-9	3.6	111
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236	Global minimum structure searches via particle swarm optimization. *Journal of Computational Chemistry*, **2007**, 28, 1177-86	3.5	111
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232	Unravelling phenomenon of internal rotation in B13+ through chemical bonding analysis. *Chemical Communications*, **2011**, 47, 6242-4	5.8	106
231	Recent developments and future prospects of all-metal aromatic compounds. *Chemical Society Reviews*, **2015**, 44, 6519-34	58.5	95
230	Photoelectron spectroscopy and ab initio study of the doubly antiaromatic B(6) (2-) dianion in the LiB(6) (-) cluster. *Journal of Chemical Physics*, **2005**, 122, 54313	3.9	92
229	Probing the structures and bonding of size-selected boron and doped-boron clusters. *Chemical Society Reviews*, **2019**, 48, 3550-3591	58.5	90
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226	Probing the Electronic Structure and Aromaticity of Pentapnictogen Cluster Anions Pn5- (Pn = P, As, Sb, and Bi) Using Photoelectron Spectroscopy and ab Initio Calculations. *Journal of Physical Chemistry A*, **2002**, 106, 5600-5606	2.8	84
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218	Post-anti-van't Hoff-Le Bel motif in atomically thin germanium-copper alloy film. *Physical Chemistry Chemical Physics*, **2015**, 17, 17545-51	3.6	65
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208	A photoelectron spectroscopy and ab initio study of the structures and chemical bonding of the B25(-) cluster. *Journal of Chemical Physics*, **2014**, 141, 034303	3.9	54
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204	Inorganic double-helix structures of unusually simple lithium-phosphorus species. *Angewandte Chemie - International Edition*, **2012**, 51, 8330-3	16.4	52
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199	Ab Initio Study of the Stabilization of Multiply Charged Anions in Water. *Journal of Physical Chemistry B*, **1998**, 102, 4205-4208	3.4	48
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188	Ab Initio investigation of the structures and stabilities of CH2N2, CHFN2, and CF2N2 isomers: Important consequences of MP2 optimizations. *Journal of Computational Chemistry*, **1992**, 13, 1066-1078	3.5	44
187	Photoelectron spectroscopy of cold hydrated sulfate clusters, SO4(2-)(H2O)n (n = 4-7): temperature-dependent isomer populations. *Journal of Physical Chemistry A*, **2009**, 113, 5567-76	2.8	43

186	A single □bond captures 3, 4 and 5 atoms. *Chemical Physics Letters*, **2004**, 388, 452-456	2.5	42
185	Vibrationally resolved photoelectron spectra of CuCN□and AgCN□and ab initio studies of the structure and bonding in CuCN. *Journal of Chemical Physics*, **2000**, 112, 3627-3632	3.9	42
184	A combined experimental and theoretical study of the neutral, cationic, and anionic Si3N cluster molecule. *Journal of Chemical Physics*, **1994**, 101, 2871-2879	3.9	42
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174	Green function calculations of ionization energies of hyperalkali molecules. *Chemical Physics Letters* , **1992**, 197, 195-199	2.5	39
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171	Peculiar All-Metal □Aromaticity of the [Au Sb] Anion in the Solid State. *Angewandte Chemie - International Edition*, **2016**, 55, 15344-15346	16.4	37
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169	Ab initio study of the silicon oxide (Si2O and Si3O) molecules. *The Journal of Physical Chemistry*, **1993**, 97, 5875-5881		37

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162	□Bonding in the [Pd4(□4-C9H9)(□4-C8H8)]+ sandwich complex. *Physical Chemistry Chemical Physics*, **2010**, 12, 12050-4	3.6	34
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157	Deciphering aromaticity in porphyrinoids via adaptive natural density partitioning. *Organic and Biomolecular Chemistry*, **2014**, 12, 6145-50	3.9	31
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144	The electronic structure and chemical bonding of aluminum acetylide: Al2C2 and Al2C2 An experimental and theoretical investigation. *Journal of Chemical Physics*, **2000**, 113, 2671-2679	3.9	28
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141	Multiple local aromaticity of nonagermanide clusters. *Chemical Science*, **2019**, 10, 5761-5765	9.4	26
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139	Photoelectron spectroscopy and Ab initio study of the structure and bonding of Al7N- and Al7N. *Journal of Physical Chemistry A*, **2008**, 112, 1873-9	2.8	25
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