Alexander Larin

List of Publications by Year
in descending order

79 papers	748 citations	516215 16 h-index	713013 21 g-index
81 all docs	81 docs citations	81 times ranked	503 citing authors

#	Article	IF	Citations
1	The Loewenstein rule: the increase in electron kinetic energy as the reason for instability of Alâ€“Oâ€“Al linkage in aluminosilicate zeolites. Physics and Chemistry of Minerals, 2013, 40, 771-780.	0.3	31
2	Induced Infrared Absorption of Molecular Oxygen Sorbed in Exchanged A Zeolites. 2. Frequency Shift Calculation. The Journal of Physical Chemistry, 1996, 100, 238-244.	2.9	28
3	Estimate of ionicity of zeolite NaA using the frequency shift values of physisorbed molecular hydrogen. Molecular Physics, 1996, 88, 1399-1410.	0.8	27
4	Method for the calculation of the vibrational frequency shift of physisorbed molecules. Application to H2 adsorbed in NaA zeolite. Journal of Chemical Physics, 1994, 101, 8130-8137.	1.2	25
5	Complex study of the activity, stability and sulfur resistance of Pd/La2O3-CeO2-Al2O3 system as monolithic catalyst for abatement of methane. Chemical Engineering Journal, 2019, 368, 865-876.	6.6	25
6	Theoretical estimate ofortho-paraseparation coefficients for H2and D2on A-type zeolites for small and medium coverage. Molecular Physics, 1992, 77, 869-891.	0.8	23
7	Theoretical analysis of the synergism in the dielectric strength for SF6/CF4 mixtures. Journal of Applied Physics, 2004, 96, 109-117.	1.1	23
8	Lower order atomic multipole moments of the oxygen atoms of â€œsmall sizeâ€•H-form aluminosilicate frameworks. Journal of Molecular Catalysis A, 2001, 168, 123-138.	4.8	21
9	Structure and the electronic and magnetic properties of LaTiO3. Physics of the Solid State, 2008, 50, 1795-1798.	0.2	21
10	Ion-Exchanged Binuclear Clusters As Active Sites of Selective Oxidation over Zeolites. Journal of Physical Chemistry C, 2009, 113, 8258-8265.	1.5	21
11	Approximation of the Mulliken-type charges for the oxygen atoms of all-siliceous zeolites. Chemical Physics Letters, 1998, 287, 169-177.	1.2	20
12	Carbonate â€œdoorâ€•in the NaKA zeolite as the reason of higher CO2 uptake relative to N2. Microporous and Mesoporous Materials, 2012, 162, 98-104.	2.2	20
13	Cumulative coordinates for approximations of high-order atomic multipole moments in aluminosilicate and aluminophosphate sieves. International Journal of Quantum Chemistry, 2001, 83, 70-85.	1.0	19
14	Interaction between probe molecules and zeolites.. Physical Chemistry Chemical Physics, 2002, 4, 2424-2433.	1.3	19
15	Oxide clusters as source of the third oxygen atom for the formation of carbonates in alkaline earth dehydrated zeolites. Journal of Catalysis, 2011, 281, 212-221.	3.1	18
16	Approximations of the Mulliken charges for the oxygen and silicon atoms of zeolite frameworks calculated with a periodic Hartree-Fock scheme. International Journal of Quantum Chemistry, 1998, 70, 993-1001.	1.0	17
17	DFT investigation of CO oxidation over Mg exchanged periodic zeolite models. Computational and Theoretical Chemistry, 2011, 964, 108-115.	1.1	16
18	Quadrupole coupling constantsCQQ for2H,27Al, and17O atoms calculated at the periodic Hartree-Fock level for understanding the geometry of H-form aluminosilicates. International Journal of Quantum Chemistry, 2001, 82, 182-192.	1.0	15

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19	Confinement in molecular sieves: The pioneering physical concepts. Journal of Molecular Catalysis A, 2009, 305, 16-23.	4.8	15
20	Approximation of Mulliken charges for the silicon atoms of all-siliceous zeolites. Solid State Sciences, 1999, 1, 201-207.	0.8	14
21	Convergence of electric field and electric field gradient versus atomic basis sets in allâ€siliceous and Mg substituted phillipsites. Journal of Computational Chemistry, 2008, 29, 2344-2358.	1.5	13
22	Mechanisms and rate of dislocation nucleation in aluminum-copper alloys near Guinier-Preston zones. Journal of Applied Physics, 2016, 120, 235106.	1.1	13
23	Influence of hydrogen bonding on the properties of water molecules adsorbed in zeolite frameworks. International Journal of Quantum Chemistry, 2003, 92, 71-84.	1.0	12
24	Cumulative coordinate technique for approximation of high atomic multipole moments of aluminophosphate sieves on the basis of electron densities calculated with DFT methods. International Journal of Quantum Chemistry, 2005, 101, 807-818.	1.0	12
25	Theoretical identification of carbonate geometry in zeolites from IR spectra. Microporous and Mesoporous Materials, 2013, 173, 15-21.	2.2	12
26	Approximation of the Mulliken charges and dipole moments of the oxygen atoms of aluminophosphate sieves. Journal of Molecular Catalysis A, 2001, 166, 73-85.	4.8	11
27	The role of water in the elastic properties of aluminosilicate zeolites: DFT investigation. Journal of Molecular Modeling, 2017, 23, 68.	0.8	11
28	Role of Distant Al Atoms in Alkaline Earth Zeolites for Stabilization of Hydroxyl Groups. Journal of Physical Chemistry C, 2012, 116, 2399-2410.	1.5	10
29	Carbonates in zeolites: Formation, properties, reactivity. International Journal of Quantum Chemistry, 2015, 115, 1709-1717.	1.0	10
30	Theoretical estimation of the vibrational perturbation of the molecular properties of hydrogen adsorbed within a zeolite A framework. Chemical Physics Letters, 1997, 274, 345-353.	1.2	9
31	Interaction between probe molecules and zeolites.. Physical Chemistry Chemical Physics, 2002, 4, 2416-2423.	1.3	9
32	Computational Differentiation of BrÃ¸nsted Acidity Induced by Alkaline Earth or Rare Earth Cations in Zeolites. Inorganic Chemistry, 2012, 51, 12165-12175.	1.9	9
33	Role of cation size for hydrogen carbonate stabilization and modification of the zeoliteâ€“CO2 interaction energy: Computational analysis in alkali Y zeolites. Microporous and Mesoporous Materials, 2016, 228, 182-195.	2.2	9
34	Carbonate-Promoted Drift of Alkali Cations in Small Pore Zeolites: Ab Initio Molecular Dynamics Study of CO₂ in NaKA Zeolite. Journal of Physical Chemistry Letters, 2019, 10, 2191-2195.	2.1	9
35	Improvement of X-ray diffraction geometries of water physisorbed in zeolites on the basis of periodic Hartree-Fock calculations. International Journal of Quantum Chemistry, 2005, 102, 971-979.	1.0	8
36	Evaluation of electric field within pores of aluminophosphate sieves. International Journal of Quantum Chemistry, 2005, 105, 839-856.	1.0	8

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37	Theoretical and experimental analyses of the synergism in the dielectric strength for C3F8âˆ•C2HF5 mixtures. Journal of Applied Physics, 2007, 101, 083306.	1.1	8
38	Theory of magnetic resonance as an orbital state probe. Physical Review B, 2009, 79, .	1.1	8
39	Ionâ€exchanged binuclear Ca₂O_{<i>X</i>} clusters, <i>X</i> = 1â€“4, as active sites of selective oxidation over MOR and FAU zeolites. Journal of Computational Chemistry, 2010, 31, 421-430.	1.5	8
40	Deblocking effect of carbonates and hydrogen carbonates in the alkali form zeolites with narrow pores. Microporous and Mesoporous Materials, 2014, 200, 35-45.	2.2	8
41	Influence of carbonate species on elastic properties of NaX and NaKX zeolites. Microporous and Mesoporous Materials, 2014, 195, 276-283.	2.2	8
42	Nucleation of dislocations in aluminum alloys with copper. Physics of the Solid State, 2015, 57, 1807-1817.	0.2	8
43	Chemical reduction of the elastic properties of zeolites: a comparison of the formation of carbonate species versus dealumination. Dalton Transactions, 2015, 44, 2703-2711.	1.6	8
44	Electrostatic potential and field approximation for aluminosilicates in cation-substituted forms. Russian Journal of Physical Chemistry A, 2007, 81, 493-509.	0.1	7
45	Influence of alkali cations on the inter-conversion of extra-framework aluminium species in dealuminated zeolites. Microporous and Mesoporous Materials, 2014, 189, 173-180.	2.2	7
46	Different limits for convergent Pd-Pd lengths in Pd slabs grown over different oxides. Structural Chemistry, 2019, 30, 489-500.	1.0	7
47	Assignment of the torsional structure of the O00 band of the electronic transition A1g â†’ B2u in van der Waals clusters of type C6H6-X (X = N2, CO2, CO). Chemical Physics Letters, 1993, 213, 619-626.	1.2	5
48	Influence of the intramolecular potential of adsorbed hydrogen on frequency shift calculations. Chemical Physics Letters, 1995, 232, 383-386.	1.2	5
49	Quick scheme for evaluation of atomic charges in arbitrary aluminophosphate sieves on the basis of electron densities calculated with DFT methods. Journal of Computational Chemistry, 2007, 28, 1695-1703.	1.5	5
50	Ab initio QM calculation of the electric field convergence versus atomic basis sets in periodic models of proton-substituted zeolites. International Journal of Quantum Chemistry, 2007, 107, 3137-3150.	1.0	5
51	Electric field convergence versus atomic basis sets in all-siliceous zeolites. Journal of Computational Chemistry, 2008, 29, 130-138.	1.5	5
52	A molecular dynamics simulation of lithium fluoride: Volume phase and nanosized particle. Russian Journal of Physical Chemistry A, 2010, 84, 48-52.	0.1	5
53	Point atomic multipole moments for simulation of electrostatic potential and field in allâ€siliceous zeolites. Journal of Computational Chemistry, 2011, 32, 2459-2473.	1.5	5
54	CO diffusion as a re-orientation mechanism in the NaY zeolite. Physical Chemistry Chemical Physics, 2017, 19, 20930-20940.	1.3	5

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55	Theoretical Analysis of Oxidative Carbonylation of Methanol: Saegusaâ€™s Scheme of Dimethylcarbonate Synthesis over Binuclear Cationic Oxo-Clusters in CuNaX Zeolite. Journal of Physical Chemistry C, 2018, 122, 5366-5375.	1.5	5
56	Internal (SiH)<i>_X</i>groups,<i>X</i>= 1â€“4, in microcrystalline hydrogenated silicon and their IR spectra on the basis of periodic DFT modelling. Molecular Physics, 2014, 112, 956-962.	0.8	4
57	Theoretical aspects of methanol carbonylation on copper-containing zeolites. Petroleum Chemistry, 2016, 56, 259-266.	0.4	4
58	Spatial and Magnetic Factors for CH₄ Oxidation on Pd Slabs in the Presence of Transition-Metal Me Cations Exchanged in Î³-Al₂O₃ Support or MeAl₂O₄ Spinels, Me = Ni, Co, Mn. Journal of Physical Chemistry C, 2020, 124, 605-615.	1.5	4
59	Structure of bi- and trinuclear clusters of aluminum ions at the cationic sites of mordenite. Journal of Structural Chemistry, 2014, 55, 583-594.	0.3	3
60	DFT modeling of plasma-assisted atomic layer deposition for Si(110) passivation: formation of boehmite-like chains as Î³-Al2O3 precursors. Theoretical Chemistry Accounts, 2016, 135, 1.	0.5	3
61	Pdâ€“MeOx/Al2O3 (Meâ€‰=â€‰Co, La, Ce) catalysts for methane combustion. Reaction Kinetics, Mechanisms and Catalysis, 2019, 126, 663-678.	0.8	3
62	Charge-ordering in La0.333Ca0.667MnO3. Physica Status Solidi C: Current Topics in Solid State Physics, 2007, 4, 1222-1225.	0.8	2
63	The cumulative coordinate method for describing the electrostatic potential and field in silica zeolite polymorphs. Russian Journal of Physical Chemistry A, 2007, 81, 2003-2015.	0.1	2
64	DFT analysis of propane cyclization over binuclear Ga-clusters in mordenite. Journal of Molecular Catalysis A, 2009, 305, 90-94.	4.8	2
65	Distributed Atomic Multipole Moments for Solving Problems of Computational Chemistry. Russian Journal of Physical Chemistry A, 2019, 93, 1880-1895.	0.1	2
66	Reconstruction and catalytic activity of hybrid Pd(100)/(111) monolayer on Î³-Al₂O₃(100) in CH₄, H₂O, and O₂ dissociation. Dalton Transactions, 2021, 50, 8863-8876.	1.6	2
67	Translational dependence of the geometry of metallic mono- and bilayers optimized on semi-ionic supports: the cases of Pd on Î³-Al₂O₃(110), monoclinic ZrO₂(001), and rutile TiO₂(001). CrystEngComm, 2021, 24, 143-155.	1.3	2
68	Linear dependence of the interaction energy on intramolecular distance for adsorbed or clustered diatomic molecules. Molecular Physics, 2000, 98, 1433-1439.	0.8	1
69	On the role of organic amine templates in the synthesis of A1PO molecular sieves: An experimental and computational study. Studies in Surface Science and Catalysis, 2006, 162, 339-346.	1.5	1
70	Ab initio calculations of the structure and dynamics of perfect and imperfect MeF crystals (Me = Rb, K,) Tj ETQq0 0 0 rgBT /Overlock 10 T	0.2	1
71	Molecular Models of the Stabilization of Bivalent Metal Cations in Zeolite Catalysts. , 2011, , 579-643.		1
72	Point charges and atomic multipole moments of Si and O in amorphous SiO2 for the estimation of the electrostatic field and potential. Journal of Structural Chemistry, 2014, 55, 398-408.	0.3	1

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73	The influence of spatial limits on the modeling chemical reactivity: The example of CO₂ hydration in MeX zeolites (Me = K, Rb, Cs). International Journal of Quantum Chemistry, 2019, 119, e25820.	1.0	1
74	Differences between the CO and NO properties for stability of alkali metal complexes Me(XO)n+, X=C or N. International Journal of Quantum Chemistry, 2002, 90, 541-548.	1.0	0
75	The ab-initio calculation of crystal structure and lattice dynamics of perfect and defective MeX (Me⁺= Rb⁺, K⁺, Na⁺; X⁻= F⁻,) Tj ETQq1 0.784314 rgBT /	0.3	0
76	Local structure and lattice dynamics of alkali halide crystals with an anion vacancy. Physics of the Solid State, 2008, 50, 1756-1760.	0.2	0
77	Detailed Atomistic Modeling of Si(110) Passivation by Atomic Layer Deposition of Al2O3. , 2016, , 303-351.		0
78	Similarities between amorphous and microcrystalline forms of hydrogenated silicon from periodic DFT modelling: coupled Siâ€“H vibrations in (SiH)X groups, X = 2â€“4. Molecular Physics, 2016, 114, 2299-2304.	0.8	0
79	Catalytic combustion of methane over Ni modified Pd/Al2O3 catalysts. Materials Today: Proceedings, 2022, , .	0.9	0