Sergey V Levchenko

List of Publications by Year
in descending order

65	8,895	172386 29	123376 61
papers	citations	h-index	g-index

67	67	67	10973
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Advances in methods and algorithms in a modern quantum chemistry program package. Physical Chemistry Chemical Physics, 2006, 8, 3172-3191.	1.3	2,597
2	Advances in molecular quantum chemistry contained in the Q-Chem 4 program package. Molecular Physics, 2015, 113, 184-215.	0.8	2,561
3	Big Data of Materials Science: Critical Role of the Descriptor. Physical Review Letters, 2015, 114, 105503.	2.9	658
4	Equation-of-motion spin-flip coupled-cluster model with single and double substitutions: Theory and application to cyclobutadiene. Journal of Chemical Physics, 2004, 120, 175-185.	1.2	293
5	Ni Single Atom Catalysts for CO₂ Activation. Journal of the American Chemical Society, 2019, 141, 2451-2461.	6.6	291
6	A Critical Assessment of Li/MgO-Based Catalysts for the Oxidative Coupling of Methane. Catalysis Reviews - Science and Engineering, 2011, 53, 424-514.	5.7	205
7	Femtosecond Multidimensional Imaging of a Molecular Dissociation. Science, 2006, 311, 219-222.	6.0	164
8	Beyond Scaling Relations for the Description of Catalytic Materials. ACS Catalysis, 2019, 9, 2752-2759.	5.5	157
9	Manyâ€Body Dispersion Interactions in Molecular Crystal Polymorphism. Angewandte Chemie - International Edition, 2013, 52, 6629-6632.	7.2	149
10	Hybrid functionals for large periodic systems in an all-electron, numeric atom-centered basis framework. Computer Physics Communications, 2015, 192, 60-69.	3.0	133
11	Discovery of Quantitative Electronic Structureâ€OER Activity Relationship in Metalâ€Organic Framework Electrocatalysts Using an Integrated Theoreticalâ€Experimental Approach. Advanced Functional Materials, 2021, 31, 2102066.	7.8	114
12	Concentration of Vacancies at Metal-Oxide Surfaces: Case Study of MgO(100). Physical Review Letters, 2013, 111, 045502.	2.9	104
13	Temperatureâ€Dependent Morphology, Magnetic and Optical Properties of Liâ€Doped MgO. ChemCatChem, 2010, 2, 854-862.	1.8	102
14	Influence of Ferroelectric Polarization on the Equilibrium Stoichiometry of Lithium Niobate (0001) Surfaces. Physical Review Letters, 2008, 100, 256101.	2.9	100
15	Learning physical descriptors for materials science by compressed sensing. New Journal of Physics, 2017, 19, 023017.	1.2	100
16	Analytic gradients for the spin-conserving and spin-flipping equation-of-motion coupled-cluster models with single and double substitutions. Journal of Chemical Physics, 2005, 122, 224106.	1.2	82
17	Towards efficient data exchange and sharing for big-data driven materials science: metadata and data formats. Npj Computational Materials, 2017, 3, .	3.5	79
18	Step-flow growth in homoepitaxy of Î²-Ga2O3 (100)â€"The influence of the miscut direction and faceting. APL Materials, 2019, 7, .	2.2	73

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19	Single-atom alloy catalysts designed by first-principles calculations and artificial intelligence. Nature Communications, 2021, 12, 1833.	5.8	73
20	Stability and Metastability of Clusters in a Reactive Atmosphere: Theoretical Evidence for Unexpected Stoichiometries of<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mi>Mg</mml:mi><mml:mi>M</mml:mi></mml:msub><mml:msub><mml:mi mathvariant="bold">O</mml:mi><mml:mi>x</mml:mi></mml:msub></mml:math>. Physical Review Letters, 2013, 111, 135501.	2.9	72
21	Coherent vibrational dynamics reveals lattice anharmonicity in organicâ€“inorganic halide perovskite nanocrystals. Nature Communications, 2021, 12, 2629.	5.8	58
22	Interaction of Water with the CaO(001) Surface. Journal of Physical Chemistry C, 2016, 120, 5565-5576.	1.5	49
23	Rigorous Definition of Oxidation States of Ions in Solids. Physical Review Letters, 2012, 108, 166403.	2.9	48
24	Artificial-intelligence-driven discovery of catalyst genes with application to CO2 activation on semiconductor oxides. Nature Communications, 2022, 13, 419.	5.8	45
25	First-principles supercell calculations of small polarons with proper account for long-range polarization effects. New Journal of Physics, 2018, 20, 033023.	1.2	43
26	Efficientab initioschemes for finding thermodynamically stable and metastable atomic structures: benchmark of cascade genetic algorithms. New Journal of Physics, 2014, 16, 123016.	1.2	37
27	Au<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mrow /><mml:mi>N</mml:mi></mml:msub></mml:math>clusters (<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML") Tj ETQq1 1 0.784314 rgBT /Overlock 10 Tf 50 422 Td (display="in on MgO(100) surfaces: Effect of exact exchange and dispersion interactions on adhesion energies. Physical Review B, 2012, 85, .	1.1	35
28	First-Principles Atomistic Thermodynamics and Configurational Entropy. Frontiers in Chemistry, 2020, 8, 757.	1.8	32
29	Modulation of the Work Function by the Atomic Structure of Strong Organic Electron Acceptors on Hâ€Si(111). Advanced Electronic Materials, 2019, 5, 1800891.	2.6	30
30	Photodissociation dynamics of the NO dimer. I. Theoretical overview of the ultraviolet singlet excited states. Journal of Chemical Physics, 2006, 125, 084301.	1.2	28
31	Formation of Water Chains on CaO(001): What Drives the 1D Growth?. Journal of Physical Chemistry Letters, 2015, 6, 1204-1208.	2.1	26
32	Theoretical evidence for unexpected O-rich phases at corners of MgO surfaces. Physical Review Materials, 2017, 1, .	0.9	24
33	Beyond Vinyl:Â Electronic Structure of Unsaturated Propen-1-yl, Propen-2-yl, 1-Buten-2-yl, andtrans-2-Buten-2-yl Hydrocarbon Radicals. Journal of Physical Chemistry A, 2006, 110, 2746-2758.	1.1	20
34	Defect complexes in Li-doped MgO. Physical Review B, 2015, 91, .	1.1	20
35	Revisiting surface core-level shifts for ionic compounds. Physical Review B, 2019, 100, .	1.1	20
36	DFT Mechanistic Study on the Complete Oxidation of Ethylene by the Silica-Supported Pt Catalyst: Cî•Ć Activation via the Ethylene Dioxide Intermediate. Journal of Physical Chemistry C, 2019, 123, 12706-12715.	1.5	19

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37	Electronic structure of halogen-substituted methyl radicals: Excited states of CH2Cl and CH2F. Journal of Chemical Physics, 2001, 115, 7485-7494.	1.2	17
38	Surface core level BE shifts for CaO(100): insights into physical origins. Physical Chemistry Chemical Physics, 2019, 21, 25431-25438.	1.3	17
39	Rydbergâ€“valence interactions in CH2Clâ†'CH2+Cl photodissociation: Dependence of absorption probability on ground state vibrational excitation. Journal of Chemical Physics, 2003, 118, 9233-9240.	1.2	15
40	CO Adsorption on GaPdâ€”Unravelling the Chemical Bonding in Real Space. ChemPhysChem, 2017, 18, 334-337.	1.0	15
41	Main-group test set for materials science and engineering with user-friendly graphical tools for error analysis: systematic benchmark of the numerical and intrinsic errors in state-of-the-art electronic-structure approximations. New Journal of Physics, 2019, 21, 013025.	1.2	15
42	Pentacene and tetracene molecules and films on H/Si(111): level alignment from hybrid density functional theory. Electronic Structure, 2020, 2, 035002.	1.0	15
43	Electronic Structure of Halogen-Substituted Methyl Radicals:Â Equilibrium Geometries and Vibrational Spectra of CH2Cl and CH2F. Journal of Physical Chemistry A, 2002, 106, 5169-5176.	1.1	14
44	Controlling CH 2 dissociation on Ru(0001) through surface site blocking by adsorbed hydrogen. Journal of Catalysis, 2014, 320, 89-96.	3.1	13
45	Ni Substitutional Defects in Bulk and at the (001) Surface of MgO from First-Principles Calculations. Journal of Physical Chemistry C, 2016, 120, 26934-26944.	1.5	12
46	Is the Abrikosov model applicable for describing electronic vortices in plasmas?. JETP Letters, 1998, 67, 482-488.	0.4	11
47	Breaking the Curse of the Non-Dynamical Correlation Problem: The Spin-Flip Method. ACS Symposium Series, 2007, , 89-102.	0.5	11
48	Stabilization of highly polarized PbTiO<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mrow /><mml:mn>3</mml:mn></mml:msub></mml:math>nanoscale capacitors due to in-plane symmetry breaking at the interface. Physical Review B, 2012, 85, .	1.1	11
49	Li/MgO Catalysts Doped with Alioâ€valent Ions. Part II: Local Topology Unraveled by EPR/NMR and DFT Modeling. ChemCatChem, 2017, 9, 3597-3610.	1.8	11
50	Strengthening goldâ€“gold bonds by complexing gold clusters with noble gases. Inorganic Chemistry Communication, 2015, 55, 153-156.	1.8	10
51	CO adsorption on the GaPd(1ì„1ì„1ì„) surface: a comparative DFT study using different functionals. Physical Chemistry Chemical Physics, 2016, 18, 14390-14400.	1.3	8
52	CH₂ Stabilized at Steps on Ru(0001) by Coadsorbates. Journal of Physical Chemistry C, 2016, 120, 24724-24733.	1.5	8
53	Structure and Electronic Properties of Transition-Metal/Mg Bimetallic Clusters at Realistic Temperatures and Oxygen Partial Pressures. Journal of Physical Chemistry C, 2018, 122, 16788-16794.	1.5	8
54	Crystallographic Orientation Dependence of Surface Segregation and Alloying on PdCu Catalysts for CO₂ Hydrogenation. Journal of Physical Chemistry Letters, 2021, 12, 2570-2575.	2.1	7

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55	Small Polarons in Two-Dimensional Pnictogens: A First-Principles Study. Journal of Physical Chemistry Letters, 2021, 12, 4674-4680.	2.1	7
56	â€œSelf-trappingâ€•in solar cell hybrid inorganic-organic perovskite absorbers. Applied Materials Today, 2022, 26, 101380.	2.3	6
57	Adatom Bonding Sites in a Nickelâ€Fe₃O₄(001) Singleâ€Atom Model Catalyst and O₂ Reactivity Unveiled by Surface Action Spectroscopy with Infrared Freeâ€Electron Laser Light. Angewandte Chemie - International Edition, 2022, 61, e202202561.	7.2	6
58	Force calculation of polyatomic molecules in quantum Monte Carlo using Pulay's corrections. Molecular Physics, 2007, 105, 2493-2497.	0.8	5
59	New Prospects for High Performance SONAR, Chemical Sensor, and Communication Device Materials. , 2009, , .		3
60	Anharmonicity in a double hydrogen transfer reaction studied in a single porphycene molecule on a Cu(110) surface. Physical Chemistry Chemical Physics, 2018, 20, 12112-12119.	1.3	3
61	First-principles study of Pd-alloyed Cu(111) surface in hydrogen atmosphere at realistic temperatures. Journal of Applied Physics, 2020, 128, 145302.	1.1	2
62	Dielectric function of six elemental metals. Journal of Physics: Conference Series, 2021, 1890, 012008.	0.3	2
63	Adatom Bonding Sites in a Nickelâ€Fe3O4(001) Singleâ€Atom Model Catalyst and O2 Reactivity Unveiled by Surface Action Spectroscopy with Infrared Freeâ€electron Laser Light. Angewandte Chemie, 0, , .	1.6	2
64	Compact representation of one-particle wavefunctions and scalar fields obtained from electronic-structure calculations. Computer Physics Communications, 2019, 237, 42-46.	3.0	0
65	Vibrational Wave-packet Dynamics Reveals Intrinsic Lattice Anharmonicity in Hybrid Perovskite Nanocrystals. , 0, , .		0