Sergey V Levchenko

List of Publications by Year in Descending Order

64 papers	7,151 citations	25 h-index	67 g-index
67 ext. papers	8,055 ext. citations	6.1 avg, IF	5.38 L-index

#	Paper	IF	Citations
64	Artificial-intelligence-driven discovery of catalyst genes with application to CO activation on semiconductor oxides.. *Nature Communications*, **2022**, 13, 419	17.4	13
63	Self-trapping in solar cell hybrid inorganic-organic perovskite absorbers. *Applied Materials Today*, **2022**, 26, 101380	6.6	0
62	Adatom Bonding Sites in a Nickel-Fe O (001) Single-Atom Model Catalyst and O Reactivity Unveiled by Surface Action Spectroscopy with Infrared Free-Electron Laser Light.. *Angewandte Chemie - International Edition*, **2022**, e202202561	16.4	0
61	Crystallographic Orientation Dependence of Surface Segregation and Alloying on PdCu Catalysts for CO Hydrogenation. *Journal of Physical Chemistry Letters*, **2021**, 12, 2570-2575	6.4	3
60	Single-atom alloy catalysts designed by first-principles calculations and artificial intelligence. *Nature Communications*, **2021**, 12, 1833	17.4	22
59	Dielectric function of six elemental metals. *Journal of Physics: Conference Series*, **2021**, 1890, 012008	0.3	
58	Small Polarons in Two-Dimensional Pnictogens: A First-Principles Study. *Journal of Physical Chemistry Letters*, **2021**, 12, 4674-4680	6.4	0
57	Coherent vibrational dynamics reveals lattice anharmonicity in organic-inorganic halide perovskite nanocrystals. *Nature Communications*, **2021**, 12, 2629	17.4	12
56	Discovery of Quantitative Electronic Structure-OER Activity Relationship in Metal-Organic Framework Electrocatalysts Using an Integrated Theoretical-Experimental Approach. *Advanced Functional Materials*, **2021**, 31, 2102066	15.6	16
55	Spin-Polarized Plasmonics: Fresh View on Magnetic Nanoparticles. *Topics in Applied Physics*, **2021**, 53-74	0.5	
54	First-Principles Atomistic Thermodynamics and Configurational Entropy. *Frontiers in Chemistry*, **2020**, 8, 757	5	8
53	First-principles study of Pd-alloyed Cu(111) surface in hydrogen atmosphere at realistic temperatures. *Journal of Applied Physics*, **2020**, 128, 145302	2.5	0
52	Pentacene and tetracene molecules and films on H/Si(111): level alignment from hybrid density functional theory. *Electronic Structure*, **2020**, 2, 035002	2.6	6
51	Revisiting surface core-level shifts for ionic compounds. *Physical Review B*, **2019**, 100,	3.3	13
50	DFT Mechanistic Study on the Complete Oxidation of Ethylene by the Silica-Supported Pt Catalyst: C?C Activation via the Ethylene Dioxide Intermediate. *Journal of Physical Chemistry C*, **2019**,	3.8	7
49	Modulation of the Work Function by the Atomic Structure of Strong Organic Electron Acceptors on H-Si(111). *Advanced Electronic Materials*, **2019**, 5, 1800891	6.4	21
48	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	2.9	10

47	Beyond Scaling Relations for the Description of Catalytic Materials. *ACS Catalysis*, **2019**, 9, 2752-2759	13.1	95
46	Surface core level BE shifts for CaO(100): insights into physical origins. *Physical Chemistry Chemical Physics*, **2019**, 21, 25431-25438	3.6	10
45	Step-flow growth in homoepitaxy of Ga2O3 (100): The influence of the miscut direction and faceting. *APL Materials*, **2019**, 7, 022515	5.7	47
44	Compact representation of one-particle wavefunctions and scalar fields obtained from electronic-structure calculations. *Computer Physics Communications*, **2019**, 237, 42-46	4.2	
43	Ni Single Atom Catalysts for CO Activation. *Journal of the American Chemical Society*, **2019**, 141, 2451-2466	14.4	162
42	First-principles supercell calculations of small polarons with proper account for long-range polarization effects. *New Journal of Physics*, **2018**, 20, 033023	2.9	25
41	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	3.6	2
40	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	3.8	7
39	Learning physical descriptors for materials science by compressed sensing. *New Journal of Physics*, **2017**, 19, 023017	2.9	72
38	Li/MgO Catalysts Doped with Alio-valent Ions. Part II: Local Topology Unraveled by EPR/NMR and DFT Modeling. *ChemCatChem*, **2017**, 9, 3597-3610	5.2	10
37	CO Adsorption on GaPd-Unravelling the Chemical Bonding in Real Space. *ChemPhysChem*, **2017**, 18, 334-337	3.2	13
36	Towards efficient data exchange and sharing for big-data driven materials science: metadata and data formats. *Npj Computational Materials*, **2017**, 3,	10.9	53
35	Theoretical evidence for unexpected O-rich phases at corners of MgO surfaces. *Physical Review Materials*, **2017**, 1,	3.2	21
34	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	3.8	9
33	CH2 Stabilized at Steps on Ru(0001) by Coadsorbates. *Journal of Physical Chemistry C*, **2016**, 120, 24724-24733	3.8	7
32	Interaction of Water with the CaO(001) Surface. *Journal of Physical Chemistry C*, **2016**, 120, 5565-5576	3.8	38
31	CO adsorption on the GaPd(1[combining macron]1[combining macron]1[combining macron]) surface: a comparative DFT study using different functionals. *Physical Chemistry Chemical Physics*, **2016**, 18, 14390-400	3.6	8
30	Hybrid functionals for large periodic systems in an all-electron, numeric atom-centered basis framework. *Computer Physics Communications*, **2015**, 192, 60-69	4.2	89

29	Big data of materials science: critical role of the descriptor. *Physical Review Letters*, **2015**, 114, 105503	7.4	495
28	Strengthening gold–gold bonds by complexing gold clusters with noble gases. *Inorganic Chemistry Communication*, **2015**, 55, 153-156	3.1	10
27	Formation of Water Chains on CaO(001): What Drives the 1D Growth?. *Journal of Physical Chemistry Letters*, **2015**, 6, 1204-8	6.4	25
26	Advances in molecular quantum chemistry contained in the Q-Chem 4 program package. *Molecular Physics*, **2015**, 113, 184-215	1.7	2068
25	Defect complexes in Li-doped MgO. *Physical Review B*, **2015**, 91,	3.3	15
24	Efficientab initioschemes for finding thermodynamically stable and metastable atomic structures: benchmark of cascade genetic algorithms. *New Journal of Physics*, **2014**, 16, 123016	2.9	33
23	Controlling CH2 dissociation on Ru(0001) through surface site blocking by adsorbed hydrogen. *Journal of Catalysis*, **2014**, 320, 89-96	7.3	11
22	Stability and metastability of clusters in a reactive atmosphere: theoretical evidence for unexpected stoichiometries of MgMOx. *Physical Review Letters*, **2013**, 111, 135501	7.4	62
21	Many-body dispersion interactions in molecular crystal polymorphism. *Angewandte Chemie - International Edition*, **2013**, 52, 6629-32	16.4	129
20	Concentration of vacancies at metal-oxide surfaces: case study of MgO(100). *Physical Review Letters*, **2013**, 111, 045502	7.4	85
19	Rigorous definition of oxidation states of ions in solids. *Physical Review Letters*, **2012**, 108, 166403	7.4	39
18	Stabilization of highly polarized PbTiO3 nanoscale capacitors due to in-plane symmetry breaking at the interface. *Physical Review B*, **2012**, 85,	3.3	11
17	AuN clusters (N=1--6) supported on MgO(100) surfaces: Effect of exact exchange and dispersion interactions on adhesion energies. *Physical Review B*, **2012**, 85,	3.3	30
16	A Critical Assessment of Li/MgO-Based Catalysts for the Oxidative Coupling of Methane. *Catalysis Reviews - Science and Engineering*, **2011**, 53, 424-514	12.6	174
15	Temperature-Dependent Morphology, Magnetic and Optical Properties of Li-Doped MgO. *ChemCatChem*, **2010**, 2, 854-862	5.2	91
14	New Prospects for High Performance SONAR, Chemical Sensor, and Communication Device Materials **2009**,		2
13	Influence of ferroelectric polarization on the equilibrium stoichiometry of lithium niobate (0001) surfaces. *Physical Review Letters*, **2008**, 100, 256101	7.4	91
12	Force calculation of polyatomic molecules in quantum Monte Carlo using Pulay's corrections. *Molecular Physics*, **2007**, 105, 2493-2497	1.7	5

11	Breaking the Curse of the Non-Dynamical Correlation Problem: The Spin-Flip Method. *ACS Symposium Series*, **2007**, 89-102	0.4	10
10	Photodissociation dynamics of the NO dimer. I. Theoretical overview of the ultraviolet singlet excited states. *Journal of Chemical Physics*, **2006**, 125, 084301	3.9	27
9	Femtosecond multidimensional imaging of a molecular dissociation. *Science*, **2006**, 311, 219-22	33.3	150
8	Beyond vinyl: electronic structure of unsaturated propen-1-yl, propen-2-yl, 1-buten-2-yl, and trans-2-buten-2-yl hydrocarbon radicals. *Journal of Physical Chemistry A*, **2006**, 110, 2746-58	2.8	19
7	Advances in methods and algorithms in a modern quantum chemistry program package. *Physical Chemistry Chemical Physics*, **2006**, 8, 3172-91	3.6	2371
6	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	3.9	76
5	Equation-of-motion spin-flip coupled-cluster model with single and double substitutions: Theory and application to cyclobutadiene. *Journal of Chemical Physics*, **2004**, 120, 175-85	3.9	269
4	Rydberg□valence interactions in CH2Cl-ĊH2+Cl photodissociation: Dependence of absorption probability on ground state vibrational excitation. *Journal of Chemical Physics*, **2003**, 118, 9233-9240	3.9	14
3	Electronic Structure of Halogen-Substituted Methyl Radicals:□Equilibrium Geometries and Vibrational Spectra of CH2Cl and CH2F. *Journal of Physical Chemistry A*, **2002**, 106, 5169-5176	2.8	14
2	Electronic structure of halogen-substituted methyl radicals: Excited states of CH2Cl and CH2F. *Journal of Chemical Physics*, **2001**, 115, 7485-7494	3.9	17
1	Is the Abrikosov model applicable for describing electronic vortices in plasmas?. *JETP Letters*, **1998**, 67, 482-488	1.2	9