

Sergey V Levchenko

List of Publications by Citations

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The third column is the impact factor (IF) of the journal, and the fourth column is the number of citations of the article.

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	Advances in methods and algorithms in a modern quantum chemistry program package. <i>Physical Chemistry Chemical Physics</i> , 2006 , 8, 3172-91	3.6	2371
63	Advances in molecular quantum chemistry contained in the Q-Chem 4 program package. <i>Molecular Physics</i> , 2015 , 113, 184-215	1.7	2068
62	Big data of materials science: critical role of the descriptor. <i>Physical Review Letters</i> , 2015 , 114, 105503	7.4	495
61	Equation-of-motion spin-flip coupled-cluster model with single and double substitutions: Theory and application to cyclobutadiene. <i>Journal of Chemical Physics</i> , 2004 , 120, 175-85	3.9	269
60	A Critical Assessment of Li/MgO-Based Catalysts for the Oxidative Coupling of Methane. <i>Catalysis Reviews - Science and Engineering</i> , 2011 , 53, 424-514	12.6	174
59	Ni Single Atom Catalysts for CO Activation. <i>Journal of the American Chemical Society</i> , 2019 , 141, 2451-2466	16.4	162
58	Femtosecond multidimensional imaging of a molecular dissociation. <i>Science</i> , 2006 , 311, 219-22	33.3	150
57	Many-body dispersion interactions in molecular crystal polymorphism. <i>Angewandte Chemie - International Edition</i> , 2013 , 52, 6629-32	16.4	129
56	Beyond Scaling Relations for the Description of Catalytic Materials. <i>ACS Catalysis</i> , 2019 , 9, 2752-2759	13.1	95
55	Temperature-Dependent Morphology, Magnetic and Optical Properties of Li-Doped MgO. <i>ChemCatChem</i> , 2010 , 2, 854-862	5.2	91
54	Influence of ferroelectric polarization on the equilibrium stoichiometry of lithium niobate (0001) surfaces. <i>Physical Review Letters</i> , 2008 , 100, 256101	7.4	91
53	Hybrid functionals for large periodic systems in an all-electron, numeric atom-centered basis framework. <i>Computer Physics Communications</i> , 2015 , 192, 60-69	4.2	89
52	Concentration of vacancies at metal-oxide surfaces: case study of MgO(100). <i>Physical Review Letters</i> , 2013 , 111, 045502	7.4	85
51	Analytic gradients for the spin-conserving and spin-flipping equation-of-motion coupled-cluster models with single and double substitutions. <i>Journal of Chemical Physics</i> , 2005 , 122, 224106	3.9	76
50	Learning physical descriptors for materials science by compressed sensing. <i>New Journal of Physics</i> , 2017 , 19, 023017	2.9	72
49	Stability and metastability of clusters in a reactive atmosphere: theoretical evidence for unexpected stoichiometries of MgMOx. <i>Physical Review Letters</i> , 2013 , 111, 135501	7.4	62
48	Towards efficient data exchange and sharing for big-data driven materials science: metadata and data formats. <i>Npj Computational Materials</i> , 2017 , 3,	10.9	53

47	Step-flow growth in homoepitaxy of Ga_2O_3 (100) – The influence of the miscut direction and faceting. <i>APL Materials</i> , 2019 , 7, 022515	5.7	47
46	Rigorous definition of oxidation states of ions in solids. <i>Physical Review Letters</i> , 2012 , 108, 166403	7.4	39
45	Interaction of Water with the $\text{CaO}(001)$ Surface. <i>Journal of Physical Chemistry C</i> , 2016 , 120, 5565-5576	3.8	38
44	Efficient algorithms for finding thermodynamically stable and metastable atomic structures: benchmark of cascade genetic algorithms. <i>New Journal of Physics</i> , 2014 , 16, 123016	2.9	33
43	AuN clusters (N=1–6) supported on $\text{MgO}(100)$ surfaces: Effect of exact exchange and dispersion interactions on adhesion energies. <i>Physical Review B</i> , 2012 , 85,	3.3	30
42	Photodissociation dynamics of the NO dimer. I. Theoretical overview of the ultraviolet singlet excited states. <i>Journal of Chemical Physics</i> , 2006 , 125, 084301	3.9	27
41	Formation of Water Chains on $\text{CaO}(001)$: What Drives the 1D Growth?. <i>Journal of Physical Chemistry Letters</i> , 2015 , 6, 1204-8	6.4	25
40	First-principles supercell calculations of small polarons with proper account for long-range polarization effects. <i>New Journal of Physics</i> , 2018 , 20, 033023	2.9	25
39	Single-atom alloy catalysts designed by first-principles calculations and artificial intelligence. <i>Nature Communications</i> , 2021 , 12, 1833	17.4	22
38	Modulation of the Work Function by the Atomic Structure of Strong Organic Electron Acceptors on $\text{H-Si}(111)$. <i>Advanced Electronic Materials</i> , 2019 , 5, 1800891	6.4	21
37	Theoretical evidence for unexpected O-rich phases at corners of MgO surfaces. <i>Physical Review Materials</i> , 2017 , 1,	3.2	21
36	Beyond vinyl: electronic structure of unsaturated propen-1-yl, propen-2-yl, 1-buten-2-yl, and trans-2-buten-2-yl hydrocarbon radicals. <i>Journal of Physical Chemistry A</i> , 2006 , 110, 2746-58	2.8	19
35	Electronic structure of halogen-substituted methyl radicals: Excited states of CH_2Cl and CH_2F . <i>Journal of Chemical Physics</i> , 2001 , 115, 7485-7494	3.9	17
34	Discovery of Quantitative Electronic Structure-OER Activity Relationship in Metal-Organic Framework Electrocatalysts Using an Integrated Theoretical-Experimental Approach. <i>Advanced Functional Materials</i> , 2021 , 31, 2102066	15.6	16
33	Defect complexes in Li-doped MgO . <i>Physical Review B</i> , 2015 , 91,	3.3	15
32	Rydberg-valence interactions in $\text{CH}_2\text{Cl}-\text{CH}_2+\text{Cl}$ photodissociation: Dependence of absorption probability on ground state vibrational excitation. <i>Journal of Chemical Physics</i> , 2003 , 118, 9233-9240	3.9	14
31	Electronic Structure of Halogen-Substituted Methyl Radicals: Equilibrium Geometries and Vibrational Spectra of CH_2Cl and CH_2F . <i>Journal of Physical Chemistry A</i> , 2002 , 106, 5169-5176	2.8	14
30	CO Adsorption on GaPd -Unravelling the Chemical Bonding in Real Space. <i>ChemPhysChem</i> , 2017 , 18, 334-337	3.7	13

29	Revisiting surface core-level shifts for ionic compounds. <i>Physical Review B</i> , 2019 , 100,	3.3	13
28	Artificial-intelligence-driven discovery of catalyst genes with application to CO activation on semiconductor oxides.. <i>Nature Communications</i> , 2022 , 13, 419	17.4	13
27	Coherent vibrational dynamics reveals lattice anharmonicity in organic-inorganic halide perovskite nanocrystals. <i>Nature Communications</i> , 2021 , 12, 2629	17.4	12
26	Controlling CH ₂ dissociation on Ru(0001) through surface site blocking by adsorbed hydrogen. <i>Journal of Catalysis</i> , 2014 , 320, 89-96	7.3	11
25	Stabilization of highly polarized PbTiO ₃ nanoscale capacitors due to in-plane symmetry breaking at the interface. <i>Physical Review B</i> , 2012 , 85,	3.3	11
24	Li/MgO Catalysts Doped with Alio-valent Ions. Part II: Local Topology Unraveled by EPR/NMR and DFT Modeling. <i>ChemCatChem</i> , 2017 , 9, 3597-3610	5.2	10
23	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. <i>New Journal of Physics</i> , 2019 , 21, 013025	2.9	10
22	Strengthening gold-gold bonds by complexing gold clusters with noble gases. <i>Inorganic Chemistry Communication</i> , 2015 , 55, 153-156	3.1	10
21	Breaking the Curse of the Non-Dynamical Correlation Problem: The Spin-Flip Method. <i>ACS Symposium Series</i> , 2007 , 89-102	0.4	10
20	Surface core level BE shifts for CaO(100): insights into physical origins. <i>Physical Chemistry Chemical Physics</i> , 2019 , 21, 25431-25438	3.6	10
19	Ni Substitutional Defects in Bulk and at the (001) Surface of MgO from First-Principles Calculations. <i>Journal of Physical Chemistry C</i> , 2016 , 120, 26934-26944	3.8	9
18	Is the Abrikosov model applicable for describing electronic vortices in plasmas?. <i>JETP Letters</i> , 1998 , 67, 482-488	1.2	9
17	First-Principles Atomistic Thermodynamics and Configurational Entropy. <i>Frontiers in Chemistry</i> , 2020 , 8, 757	5	8
16	CO adsorption on the GaPd(1[combining macron]1[combining macron]1[combining macron]) surface: a comparative DFT study using different functionals. <i>Physical Chemistry Chemical Physics</i> , 2016 , 18, 14390-400	3.6	8
15	DFT Mechanistic Study on the Complete Oxidation of Ethylene by the Silica-Supported Pt Catalyst: C ₂ C Activation via the Ethylene Dioxide Intermediate. <i>Journal of Physical Chemistry C</i> , 2019 ,	3.8	7
14	CH ₂ Stabilized at Steps on Ru(0001) by Coadsorbates. <i>Journal of Physical Chemistry C</i> , 2016 , 120, 24724-24733	3.8	7
13	Structure and Electronic Properties of Transition-Metal/Mg Bimetallic Clusters at Realistic Temperatures and Oxygen Partial Pressures. <i>Journal of Physical Chemistry C</i> , 2018 , 122, 16788-16794	3.8	7
12	Pentacene and tetracene molecules and films on H/Si(111): level alignment from hybrid density functional theory. <i>Electronic Structure</i> , 2020 , 2, 035002	2.6	6

11	Force calculation of polyatomic molecules in quantum Monte Carlo using Pulay's corrections. <i>Molecular Physics</i> , 2007 , 105, 2493-2497	1.7	5
10	Crystallographic Orientation Dependence of Surface Segregation and Alloying on PdCu Catalysts for CO Hydrogenation. <i>Journal of Physical Chemistry Letters</i> , 2021 , 12, 2570-2575	6.4	3
9	Anharmonicity in a double hydrogen transfer reaction studied in a single porphycene molecule on a Cu(110) surface. <i>Physical Chemistry Chemical Physics</i> , 2018 , 20, 12112-12119	3.6	2
8	New Prospects for High Performance SONAR, Chemical Sensor, and Communication Device Materials 2009 ,		2
7	First-principles study of Pd-alloyed Cu(111) surface in hydrogen atmosphere at realistic temperatures. <i>Journal of Applied Physics</i> , 2020 , 128, 145302	2.5	0
6	Self-trapping in solar cell hybrid inorganic-organic perovskite absorbers. <i>Applied Materials Today</i> , 2022 , 26, 101380	6.6	0
5	Small Polarons in Two-Dimensional Pnictogens: A First-Principles Study. <i>Journal of Physical Chemistry Letters</i> , 2021 , 12, 4674-4680	6.4	0
4	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.. <i>Angewandte Chemie - International Edition</i> , 2022 , e202202561	16.4	0
3	Dielectric function of six elemental metals. <i>Journal of Physics: Conference Series</i> , 2021 , 1890, 012008	0.3	
2	Compact representation of one-particle wavefunctions and scalar fields obtained from electronic-structure calculations. <i>Computer Physics Communications</i> , 2019 , 237, 42-46	4.2	
1	Spin-Polarized Plasmonics: Fresh View on Magnetic Nanoparticles. <i>Topics in Applied Physics</i> , 2021 , 53-74	0.5	