lev Kantorovich

List of Publications by Year
in descending order

232 papers	6,745 citations	50276 46 h-index	85541 71 g-index
236 all docs	236 docs citations	236 times ranked	4583 citing authors

#	Article	IF	Citations
1	Growth of epitaxial graphene: Theory and experiment. Physics Reports, 2014, 542, 195-295.	25.6	228
2	Atomically resolved edges and kinks of NaCl islands on Cu(111): Experiment and theory. Physical Review B, 2000, 62, 2074-2084.	3.2	213
3	The energetics and electronic structure of defective and irregular surfaces on MgO. Surface Science, 1995, 343, 221-239.	1.9	186
4	Influence of gradient corrections on the bulk and surface properties ofTiO2andSnO2. Physical Review B, 1996, 53, 957-960.	3.2	166
5	Spectroscopy of low-coordinated surface sites:â€,Theoretical study of MgO. Physical Review B, 1999, 59, 2417-2430.	3.2	164
6	Elementary Structural Motifs in a Random Network of Cytosine Adsorbed on a Gold(111) Surface. Science, 2008, 319, 312-315.	12.6	157
7	The structure of the stoichiometric and reduced SnO2(110) surface. Surface Science, 1995, 339, 258-271.	1.9	142
8	Mapping the force field of a hydrogen-bonded assembly. Nature Communications, 2014, 5, 3931.	12.8	133
9	General Theory of Microscopic Dynamical Response in Surface Probe Microscopy: From Imaging to Dissipation. Physical Review Letters, 2004, 93, 236102.	7.8	130
10	Melamine Structures on the Au(111) Surface. Journal of Physical Chemistry C, 2008, 112, 11476-11480.	3.1	122
11	Elimination of the long-range dipole interaction in calculations with periodic boundary conditions. Physical Review B, 1999, 60, 15476-15479.	3.2	119
12	Study of the surface electronic structure of MgO bulk crystals and thin films. Surface Science, 1996, 365, 557-571.	1.9	116
13	Role of van der Waals interaction in forming molecule-metal junctions: flat organic molecules on the Au(111) surface. Physical Chemistry Chemical Physics, 2010, 12, 4759.	2.8	109
14	Sublattice Identification in Scanning Force Microscopy on Alkali Halide Surfaces. Physical Review Letters, 2004, 92, 146103.	7.8	102
15	Probing the Hierarchy of Thymineâ€“Thymine Interactions in Selfâ€Assembled Structures by Manipulation with Scanning Tunneling Microscopy. Small, 2007, 3, 2011-2014.	10.0	101
16	An Investigation into the Interactions Between Selfâ€Assembled Adenine Molecules and a Au(111) Surface. Small, 2008, 4, 1494-1500.	10.0	98
17	Bond Breaking Coupled with Translation in Rolling of Covalently Bound Molecules. Physical Review Letters, 2005, 94, 146104.	7.8	85
18	Ab initio Hartreeâ€“Fock perturbedâ€cluster treatment of local defects in crystals. Journal of Chemical Physics, 1990, 92, 7448-7460.	3.0	82

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19	Pressure-inducedB1-B2 phase transition in alkali halides: General aspects from first-principles calculations. Physical Review B, 1994, 49, 3066-3074.	3.2	82
20	Adsorption of atomic and molecular oxygen on the MgO (001) surface. Surface Science, 1997, 374, 373-386.	1.9	79
21	Mg clusters on MgO surfaces: study of the nucleation mechanism with MIES and ab initio calculations. Faraday Discussions, 1999, 114, 173-194.	3.2	77
22	Toggling Bistable Atoms via Mechanical Switching of Bond Angle. Physical Review Letters, 2011, 106, 136101.	7.8	77
23	Two-Dimensional Supramolecular Nanopatterns Formed by the Coadsorption of Guanine and Uracil at the Liquid/Solid Interface. Journal of the American Chemical Society, 2008, 130, 695-702.	13.7	72
24	Specificity of Watsonâ€“Crick Base Pairing on a Solid Surface Studied at the Atomic Scale. Angewandte Chemie - International Edition, 2008, 47, 9673-9676.	13.8	71
25	Calculations of the geometry and optical properties ofFMgcenters and dimer (F2-type) centers in corundum crystals. Physical Review B, 1995, 51, 8770-8778.	3.2	70
26	Adenine monolayers on the Au(111) surface: Structure identification by scanning tunneling microscopy experiment and ab initio calculations. Journal of Chemical Physics, 2009, 130, 024705.	3.0	68
27	Homopairing Possibilities of the DNA Base Adenine. Journal of Physical Chemistry B, 2005, 109, 11933-11939.	2.6	67
28	Prochiral Guanine Adsorption on Au(111): An Entropyâ€Stabilized Intermixed Guanineâ€Quartet Chiral Structure. Small, 2009, 5, 1952-1956.	10.0	65
29	Quantum-chemical simulation of impurity-induced trapping of a hole: (Li)0centre in MgO. Journal of Physics C: Solid State Physics, 1986, 19, 4183-4199.	1.5	62
30	Ionic and electronic processes at ionic surfaces induced by atomic-force-microscope tips. Physical Review B, 1997, 56, 15332-15344.	3.2	62
31	Generalized Langevin equation for solids. I. Rigorous derivation and main properties. Physical Review B, 2008, 78, .	3.2	62
32	An ab initio study of C60 adsorption on the Si(001) surface. Surface Science, 2005, 591, 45-55.	1.9	60
33	An embedded-molecular-cluster method for calculating the electronic structure of point defects in non-metallic crystals. I. General theory. Journal of Physics C: Solid State Physics, 1988, 21, 5041-5056.	1.5	58
34	Understanding the disorder of the DNA base cytosine on the Au(111) surface. Journal of Chemical Physics, 2008, 129, 184707.	3.0	57
35	H-Bonding Supramolecular Assemblies of PTCDI Molecules on the Au(111) Surface. Journal of Physical Chemistry C, 2009, 113, 21840-21848.	3.1	56
36	Precise Orientation of a Single<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mi mathvariant="normal">C</mml:mi><mml:mn>60</mml:mn></mml:msub></mml:math>Molecule on the Tip of a Scanning Probe Microscope. Physical Review Letters, 2012, 108, 268302.	7.8	55

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37	Generalized Langevin equation: An efficient approach to nonequilibrium molecular dynamics of open systems. Physical Review B, 2014, 89, .	3.2	54
38	Generalized Langevin equation for solids. II. Stochastic boundary conditions for nonequilibrium molecular dynamics simulations. Physical Review B, 2008, 78, .	3.2	53
39	Experimental and theoretical analysis of H-bonded supramolecular assemblies of PTCDA molecules. Physical Review B, 2010, 81, .	3.2	53
40	Role of image forces in non-contact scanning force microscope images of ionic surfaces. Surface Science, 2000, 445, 283-299.	1.9	52
41	Planar nucleic acid base super-structures. Journal of Materials Chemistry, 2006, 16, 1894.	6.7	52
42	Origin ofp(2Ã—1)Phase on Si(001) by Noncontact Atomic Force Microscopy at 5ÂK. Physical Review Letters, 2006, 96, 106104.	7.8	52
43	Measurement and Manipulation of the Charge State of an Adsorbed Oxygen Adatom on the Rutile TiO₂(110)-1Ã—1 Surface by nc-AFM and KPFM. Journal of the American Chemical Society, 2018, 140, 15668-15674.	13.7	51
44	Homopairing Possibilities of the DNA Bases Cytosine and Guanine:Â An ab Initio DFT Study. Journal of Physical Chemistry B, 2005, 109, 22045-22052.	2.6	49
45	Coexistence of Homochiral and Heterochiral Adenine Domains at the Liquid/Solid Interface. Journal of Physical Chemistry B, 2007, 111, 12048-12052.	2.6	48
46	Homopairing Possibilities of the DNA Base Thymine and the RNA Base Uracil:Â An ab Initio Density Functional Theory Study. Journal of Physical Chemistry B, 2006, 110, 2249-2255.	2.6	46
47	Experimental and theoretical identification of adenine monolayers on Ag-terminated Si(111). Physical Review B, 2006, 73, .	3.2	46
48	Supramolecular Porous Network Formed by Molecular Recognition between Chemically Modified Nucleobases Guanine and Cytosine. Angewandte Chemie - International Edition, 2010, 49, 9373-9377.	13.8	45
49	Quantum Theory of the Solid State: An Introduction. , 2004, , .		45
50	Thermoelastic properties of perfect crystals with nonprimitive lattices. I. General theory. Physical Review B, 1995, 51, 3520-3534.	3.2	44
51	Ionic solids at elevated temperatures and high pressures: MgF2. Journal of Chemical Physics, 1997, 107, 4337-4344.	3.0	41
52	Long-range ordered and atomic-scale control of graphene hybridization by photocycloaddition. Nature Chemistry, 2020, 12, 1035-1041.	13.6	41
53	Electrostatic energy calculation for the interpretation of scanning probe microscopy experiments. Journal of Physics Condensed Matter, 2000, 12, 795-814.	1.8	39
54	Controlled Manipulation of Atoms in Insulating Surfaces with the Virtual Atomic Force Microscope. Physical Review Letters, 2007, 98, 028101.	7.8	39

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55	Theoretical study of melamine superstructures and their interaction with the Au(111) surface. Nanotechnology, 2008, 19, 465704.	2.6	39
56	Probing theSi(001)surface with a Si tip: Anab initiostudy. Physical Review B, 2006, 73, .	3.2	38
57	Current through a multilead nanojunction in response to an arbitrary time-dependent bias. Physical Review B, 2015, 91, .	3.2	38
58	Tip-Induced Control of Charge and Molecular Bonding of Oxygen Atoms on the Rutile TiO₂ (110) Surface with Atomic Force Microscopy. ACS Nano, 2019, 13, 6917-6924.	14.6	35
59	Formation Mechanism for a Hybrid Supramolecular Network Involving Cooperative Interactions. Physical Review Letters, 2012, 108, 176103.	7.8	34
60	Temperature control in molecular dynamic simulations of non-equilibrium processes. Journal of Physics Condensed Matter, 2010, 22, 074205.	1.8	33
61	Atomic corrugation in nc-AFM of alkali halides. Applied Surface Science, 2002, 188, 232-237.	6.1	32
62	Vertical atomic manipulation with dynamic atomic-force microscopy without tip change via a multi-step mechanism. Nature Communications, 2014, 5, 4476.	12.8	32
63	Hexagonal adenine networks constructed from their homopairings. Surface Science, 2005, 589, 139-152.	1.9	30
64	Molecular dynamics simulations of atomic scale processes at close approach in non-contact atomic force microscopy. Nanotechnology, 2005, 16, S79-S84.	2.6	30
65	Driving Forces for Covalent Assembly of Porphyrins by Selective Câ€“H Bond Activation and Intermolecular Coupling on a Copper Surface. Journal of the American Chemical Society, 2016, 138, 5837-5847.	13.7	30
66	Multiscale model of the manipulation of single atoms on insulating surfaces using an atomic force microscope tip. Physical Review B, 2007, 76, .	3.2	29
67	Intramolecular bonds resolved on a semiconductor surface. Physical Review B, 2014, 90, .	3.2	29
68	Role of orbital overlap in atomic manipulation. Physical Review B, 2012, 85, .	3.2	28
69	Ethylene decomposition on Ir(111): initial path to graphene formation. Physical Chemistry Chemical Physics, 2016, 18, 27897-27909.	2.8	28
70	The prediction of metastable impact electronic spectra (MIES): perfect and defective MgO(001) surfaces by state-of-the-art methods. Surface Science, 2000, 444, 31-51.	1.9	27
71	An Endergonic Synthesis of Single Sondheimerâ€“Wong Diyne by Local Probe Chemistry. Angewandte Chemie - International Edition, 2020, 59, 10842-10847.	13.8	27
72	Quantum chemical simulations of hole self-trapping in semi-ionic crystals. International Journal of Quantum Chemistry, 1994, 52, 1177-1198.	2.0	26

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73	Atomistic simulations of the adhesion hysteresis mechanism of atomic scale dissipation in non-contact atomic force microscopy. Nanotechnology, 2004, 15, S34-S39.	2.6	26
74	Adsorption of C60on the Si(001) surface calculated within the generalized gradient approximation. Nanotechnology, 2004, 15, S1-S4.	2.6	26
75	Modelling atomic scale manipulation with the non-contact atomic force microscope. Nanotechnology, 2006, 17, 5866-5874.	2.6	26
76	Dynamical processes at oxide surfaces studied with the virtual atomic force microscope. Physical Review B, 2007, 76, .	3.2	26
77	A Small Molecule Walks Along a Surface Between Porphyrin Fences That Are Assembled Inâ€…Situ. Angewandte Chemie - International Edition, 2015, 54, 7101-7105.	13.8	26
78	Calculation of energies of radiative tunneling transitions between defects in alkali halides. Solid State Communications, 1982, 42, 749-752.	1.9	25
79	A novel approach for constructing symmetryâ€adapted basis sets for quantumâ€chemical calculations. I. Real symmetryâ€adapted orbitals. Physica Status Solidi (B): Basic Research, 1992, 174, 79-90.	1.5	25
80	Modelling of oxide surfaces. Current Opinion in Solid State and Materials Science, 1996, 1, 820-826.	11.5	25
81	Adsorption of atomic oxygen on the MgO (100) surface. Journal of the Chemical Society, Faraday Transactions, 1996, 92, 2075.	1.7	25
82	Coulomb potential inside a large finite crystal. Journal of Physics Condensed Matter, 1999, 11, 6159-6168.	1.8	25
83	Physical dissipation mechanisms in non-contact atomic force microscopy. Nanotechnology, 2004, 15, S44-S48.	2.6	25
84	Interstitial oxygen in Si andSi1â^'xGex. Physical Review B, 2004, 69, .	3.2	25
85	Dihydride dimer structures on the Si(100):H surface studied by low-temperature scanning tunneling microscopy. Physical Review B, 2008, 78, .	3.2	25
86	The energetics of N2O dissociation on CaO(001). Surface Science, 1997, 376, 169-176.	1.9	24
87	Investigating the effects of silicon tip contamination in noncontact scanning force microscopy (SFM). Applied Surface Science, 1999, 144-145, 608-612.	6.1	24
88	A simple non-equilibrium theory of non-contact dissipation force microscopy. Journal of Physics Condensed Matter, 2001, 13, 945-958.	1.8	24
89	Partition-free theory of time-dependent current correlations in nanojunctions in response to an arbitrary time-dependent bias. Physical Review B, 2017, 95, .	3.2	24
90	Models of atomic scale contrast in dissipation images of binary ionic surfaces in non-contact atomic force microscopy. Nanotechnology, 2006, 17, S205-S212.	2.6	23

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91	Modelling the manipulation of C₆₀on the Si(001) surface performed with NC-AFM. Nanotechnology, 2009, 20, 135706.	2.6	23
92	An embedded-molecular-cluster method for calculating the electronic structure of point defects in non-metallic crystals. II. Structural elements in the form of molecules. Journal of Physics C: Solid State Physics, 1988, 21, 5057-5073.	1.5	22
93	Theoretical simulation of VK-centre migration in KCl. I. A quantum-chemical study. Journal of Physics Condensed Matter, 1992, 4, 7417-7428.	1.8	22
94	Identifying passivated dynamic force microscopy tips on H:Si(100). Applied Physics Letters, 2012, 100, .	3.3	22
95	Chemical tip fingerprinting in scanning probe microscopy of an oxidized Cu(110) surface. Physical Review B, 2012, 86, .	3.2	21
96	Applications of the generalized Langevin equation: Towards a realistic description of the baths. Physical Review B, 2015, 91, .	3.2	21
97	Planar Heteropairing Possibilities of the DNA and RNA Bases:â€‰ An ab Initio Density Functional Theory Study. Journal of Physical Chemistry C, 2007, 111, 3883-3892.	3.1	20
98	Xanthine Quartets on Au(111). Journal of the American Chemical Society, 2018, 140, 54-57.	13.7	20
99	The study of thermoluminescence using the contact method of sample heating. Journal Physics D: Applied Physics, 1984, 17, 2097-2014.	2.8	19
100	Tip models and force definitions in molecular dynamics simulations of scanning force microscopy. Surface Science, 2003, 540, 497-503.	1.9	19
101	Stochastic mechanism of energy dissipation in noncontact atomic force microscopy studied using molecular dynamics with Langevin boundary conditions. Physical Review B, 2004, 70, .	3.2	19
102	Manipulation ofC60on theSi(001)surface: Experiment and theory. Physical Review B, 2006, 74, .	3.2	19
103	Is atomic-scale dissipation in NC-AFM real? Investigation using virtual atomic force microscopy. Nanotechnology, 2007, 18, 084017.	2.6	19
104	Manipulating Si(100) at 5 K using qPlus frequency modulated atomic force microscopy: Role of defects and dynamics in the mechanical switching of atoms. Physical Review B, 2011, 84, .	3.2	19
105	Homochiral Xanthine Quintet Networks Self-Assembled on Au(111) Surfaces. ACS Nano, 2011, 5, 6651-6660.	14.6	18
106	Theoretical analysis of hole self-trapping in ionic solids: Application to the KCl crystal. Physical Review B, 1993, 47, 14875-14885.	3.2	17
107	Thermoelastic properties of perfect crystals with nonprimitive lattices. II. Application to KCl and NaCl. Physical Review B, 1995, 51, 3535-3548.	3.2	17
108	Treating periodic systems using embedding: Adams-Gilbert approach. Physical Review B, 2007, 76, .	3.2	17

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109	Fabrication of a Complex Two-Dimensional Adenineâ€“Perylene-3,4,9,10-tetracarboxylic Dianhydride Chiral Nanoarchitecture through Molecular Self-Assembly. Journal of Physical Chemistry C, 2012, 116, 2493-2499.	3.1	17
110	Graphene growth by molecular beam epitaxy: an interplay between desorption, diffusion and intercalation of elemental C species on islands. Nanoscale, 2018, 10, 7396-7406.	5.6	17
111	Multipole Theory of the Polarization of Solids by Point Defects. I. Dipole Approximation. Physica Status Solidi (B): Basic Research, 1983, 120, 77-86.	1.5	16
112	Molecular processes on oxide surfaces studied by first-principles calculations. Mineralogical Magazine, 1998, 62, 669-685.	1.4	16
113	Non-contact AFM images of a C60 molecule adsorbed on the Si(001) surface: An ab initio method. Surface Science, 2006, 600, 551-558.	1.9	16
114	Partitioning scheme for density functional calculations of extended systems. Journal of Chemical Physics, 2009, 130, 144104.	3.0	16
115	Atomic-scale control of hydrogen bonding on a bare Si(100)-2<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mo>Ã—</mml:mo></mml:math>1 surface. Physical Review B, 2012, 86, .	3.2	16
116	Identifying tips for intramolecular NC-AFM imaging via in situ fingerprinting. Scientific Reports, 2014, 4, 6678.	3.3	16
117	Ostwald ripening of binary alloy particles. Journal of Chemical Physics, 2011, 134, 024521.	3.0	15
118	A diagram technique for nonorthogonal electron group functions. I. Right coset decomposition of symmetric group. Journal of Chemical Physics, 1992, 96, 8420-8426.	3.0	14
119	Pulling the<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mi mathvariant="normal">C</mml:mi><mml:mn>60</mml:mn></mml:msub></mml:math>molecule on a Si(001) surface with an STM tip: A theoretical study. Physical Review B, 2008, 77, .	3.2	14
120	Theoretical modelling of tip effects in the pushing manipulation of C₆₀on the Si(001) surface. Nanotechnology, 2008, 19, 235702.	2.6	14
121	Structure of the indium-rich InSb(001) surface. Physical Review B, 2010, 82, .	3.2	14
122	Nonequilibrium processes from generalized Langevin equations: Realistic nanoscale systems connected to two thermal baths. Physical Review B, 2016, 93, .	3.2	14
123	Fluctuating-bias controlled electron transport in molecular junctions. Physical Review B, 2016, 93, .	3.2	14
124	Partition-free approach to open quantum systems in harmonic environments: An exact stochastic Liouville equation. Physical Review B, 2017, 95, .	3.2	14
125	Interpretation of atomic friction experiments based on atomistic simulations. Journal of Vacuum Science & Technology B, 2007, 25, 1547.	1.3	13
126	Simulating system dynamics with arbitrary time step. Physical Review B, 2007, 75, .	3.2	13

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127	Construction of atomic-scale logic gates on a surface of hydrogen passivated germanium. Microelectronic Engineering, 2013, 109, 262-265.	2.4	13
128	Multipole Theory of the Polarization of Solids by Point Defects. II. The Point Charge Approximation. Physica Status Solidi (B): Basic Research, 1984, 123, 325-334.	1.5	12
129	Structure and Spectroscopy of Surface Defects from Scanning Force Microscopy: Theoretical Predictions. Physical Review Letters, 2000, 85, 3846-3849.	7.8	12
130	Comparison of localization procedures for applications in crystal embedding. Physical Review B, 2004, 70, .	3.2	12
131	Calculation of the current response in a nanojunction for an arbitrary time-dependent bias: application to the molecular wire. Journal of Physics: Conference Series, 2016, 696, 012017.	0.4	12
132	Onâ€Surface Decarboxylation Coupling Facilitated by Lockâ€toâ€Unlock Variation of Molecules upon the Reaction. Angewandte Chemie - International Edition, 2021, 60, 17435-17439.	13.8	12
133	Derivation of atomistic models for lattices consisting of weakly overlapping structural elements. International Journal of Quantum Chemistry, 2000, 78, 306-330.	2.0	11
134	Application of the non-equilibrium statistical operator method (NESOM) to dissipation atomic force microscopy. Journal of Physics Condensed Matter, 2001, 13, 1439-1459.	1.8	11
135	Energy dissipation above plane terraces of a model crystal in non-contact atomic force microscopy. Journal of Physics Condensed Matter, 2002, 14, 4329-4343.	1.8	11
136	Complex design of dissipation signals in non-contact atomic force microscopy. Physical Chemistry Chemical Physics, 2012, 14, 16250.	2.8	11
137	Dynamical behavior of a dangling bond dimer on a hydrogenated semiconductor: Ge(001):H. Physical Review B, 2015, 92, .	3.2	11
138	Formation of Hypoxanthine Tetrad by Reaction with Sodium Chloride: From Planar to Stereo. Angewandte Chemie - International Edition, 2018, 57, 16015-16019.	13.8	11
139	A theoretical description of complex thermoluminescence curves. I. Journal Physics D: Applied Physics, 1988, 21, 1008-1014.	2.8	10
140	Diagram technique for nonorthogonal electron group functions. II. Reduced density matrices and total energy. Journal of Chemical Physics, 1992, 96, 8427-8438.	3.0	10
141	Mg clusters on MgO surfaces: characterization by MIES and electronic structure ab initio calculations. Nuclear Instruments & Methods in Physics Research B, 1999, 157, 162-166.	1.4	10
142	Application of the group function theory to infinite systems. International Journal of Quantum Chemistry, 2000, 76, 511-534.	2.0	10
143	Self-Assembly of Artificial Nucleobase 1H-Benzimidazole-4,7-dione at the Liquid/Solid Interface. Journal of Physical Chemistry B, 2009, 113, 8675-8681.	2.6	10
144	Guanine Assemblies on the Au(111) Surface: A Theoretical Study. Journal of Physical Chemistry C, 2013, 117, 5684-5692.	3.1	10

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145	Critical Importance of van der Waals Stabilization in Strongly Chemically Bonded Surfaces: Cu(110):O. Journal of Chemical Theory and Computation, 2013, 9, 5578-5584.	5.3	10
146	Grapheneâ€Like Covalent Organic Framework with a Wide Band Gap Synthesized On Surface via Stepwise Reactions. Angewandte Chemie - International Edition, 2020, 59, 15958-15962.	13.8	10
147	Electron dynamics of tip-tunable oxygen species on TiO2 surface. Communications Materials, 2021, 2, .	6.9	10
148	Tip and surface properties from the distance dependence of tipâ€“surface interactions. Applied Physics A: Materials Science and Processing, 2001, 72, S59-S62.	2.3	9
149	Electron density of periodic systems derived from non-orthogonal localized orbitals. Journal of Physics Condensed Matter, 2004, 16, 2575-2584.	1.8	9
150	The role of isomerization in the kinetics of self-assembly: p-terphenyl-m-dicarbonitrile on the Ag(111) surface. Physical Chemistry Chemical Physics, 2015, 17, 11182-11192.	2.8	9
151	Simulated structure and imaging of NTCDI on Si(1 1 1)-7 Ã— 7â€‰:â€‰a combined STM, NC-AFM and DFT study. Journal of Physics Condensed Matter, 2015, 27, 054004.	1.8	9
152	A free energy study of carbon clusters on Ir(111): Precursors to graphene growth. Journal of Chemical Physics, 2017, 146, 044702.	3.0	9
153	Mechanisms of Covalent Dimerization on a Bulk Insulating Surface. Journal of Physical Chemistry C, 2017, 121, 10053-10062.	3.1	9
154	Spectroscopic Fingerprints of Carbon Monomers and Dimers on Ir(111): Experiment and Theory. Journal of Physical Chemistry C, 2017, 121, 11335-11345.	3.1	9
155	Nonadiabatic dynamics of electrons and atoms under nonequilibrium conditions. Physical Review B, 2018, 98, .	3.2	9
156	Theory of Energy Dissipation into Surface Vibrations. Nanoscience and Technology, 2002, , 371-394.	1.5	9
157	Multipole Theory of the Polarization of Solids by Point Defects. III. Transition Energy Calculations, the Approximation of Nonâ€Point Charges. Physica Status Solidi (B): Basic Research, 1986, 137, 229-240.	1.5	8
158	Quantum theory of energy dissipation in non-contact atomic force microscopy in Markovian approximation. Surface Science, 2002, 521, 117-128.	1.9	8
159	Exact calculation of the tip friction within the harmonic model. Applied Surface Science, 2003, 210, 27-31.	6.1	8
160	Nonequilibrium statistical mechanics of classical nuclei interacting with the quantum electron gas. Physical Review B, 2007, 76, .	3.2	8
161	Comparative Theoretical Study of O- and S-Containing Hydrogen-Bonded Supramolecular Structures. Journal of Physical Chemistry C, 2008, 112, 17340-17350.	3.1	8
162	Vertical manipulation of a molecule with chemical forces. Physical Review B, 2008, 77, .	3.2	8

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163	Image formation and contrast inversion in noncontact atomic force microscopy imaging of oxidized Cu(110) surfaces. Physical Review B, 2014, 90, .	3.2	8
164	c-number quantum generalized Langevin equation for an open system. Physical Review B, 2016, 94, .	3.2	8
165	Driving spin-boson models from equilibrium using exact quantum dynamics. Physical Review B, 2018, 97, .	3.2	8
166	Non-equilibrium dynamics of a classical tip interacting with a quantum surface. Journal of Physics Condensed Matter, 2002, 14, 7123-7133.	1.8	7
167	Constrained Molecular Manipulation Mediated by Attractive and Repulsive Tipâ€“Adsorbate Forces. Small, 2008, 4, 765-769.	10.0	7
168	Architecture of PTCDA molecular structures on a reconstructed InSb(001) surface. Physical Review B, 2011, 83, .	3.2	7
169	Density functional calculations of extended, periodic systems using Coulomb corrected molecular fractionation with conjugated caps method (CC-MFCC). Physical Chemistry Chemical Physics, 2014, 16, 21252-21270.	2.8	7
170	Increasing the Templating Effect on a Bulk Insulator Surface: From a Kinetically Trapped to a Thermodynamically More Stable Structure. Journal of Physical Chemistry C, 2016, 120, 17546-17554.	3.1	7
171	On-surface synthesis on a bulk insulator surface. Journal of Physics Condensed Matter, 2018, 30, 133001.	1.8	7
172	Chemical shielding of H2O and HF encapsulated inside a C60 cage. Communications Chemistry, 2021, 4, .	4.5	7
173	A theoretical description of complex thermoluminescence curves. II. Method of integral equation. Journal Physics D: Applied Physics, 1989, 22, 817-824.	2.8	6
174	Meta-Positioning of Carbonitrile Functional Groups Induces Interfacial Edge-On Phase of Oligophenyl Derivatives. Journal of Physical Chemistry C, 2014, 118, 2622-2633.	3.1	6
175	Building Motifs during Self-Assembly of para-Terphenyl-meta-dicarbonitrile on a Metal Surface: A Gas-Phase Study. Journal of Physical Chemistry C, 2014, 118, 10358-10365.	3.1	6
176	Nonequilibrium generalised Langevin equation for the calculation of heat transport properties in model 1D atomic chains coupled to two 3D thermal baths. Journal of Chemical Physics, 2017, 146, 164103.	3.0	6
177	Hydrocarbon decomposition kinetics on the Ir(111) surface. Physical Chemistry Chemical Physics, 2018, 20, 6083-6099.	2.8	6
178	Kinetic control of molecular assembly on surfaces. Communications Chemistry, 2018, 1, .	4.5	6
179	Controlling the preferential motion of chiral molecular walkers on a surface. Chemical Science, 2019, 10, 5864-5874.	7.4	6
180	Quadruped Molecular Anchoring to an Insulator: Functionalized Ferrocene on CaF₂ Bulk and Thin Film Surfaces. Journal of Physical Chemistry C, 2020, 124, 9900-9907.	3.1	6

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