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	Atomistic insight into the formation dynamics of charged point defects: A classical molecular dynamics study of F+ -centers in NaCl. Physical Review Materials, 2022, 6, .	2.4	1
2	Superâ€robust Xanthineâ€Sodium Complexes on Au(111). Angewandte Chemie - International Edition, 2022, , .	13.8	1
3	Charge State Tristability of Oxygen Adatom on a Rutile TiO₂(110)â€"(1 Ã— 1) Surface Controlled by Atomic Force Microscopy. Journal of Physical Chemistry C, 2022, 126, 5064-5069.	3.1	4
4	Quantum interference and the time-dependent radiation of nanojunctions. Physical Review B, 2021, 103, .	3.2	6
5	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
6	Onâ€Surface Decarboxylation Coupling Facilitated by Lockâ€toâ€Unlock Variation of Molecules upon the Reaction. Angewandte Chemie, 2021, 133, 17575-17579.	2.0	2
7	Electron dynamics of tip-tunable oxygen species on TiO2 surface. Communications Materials, 2021, 2, .	6.9	10
8	Chemical shielding of H2O and HF encapsulated inside a C60 cage. Communications Chemistry, 2021, 4, .	4.5	7
9	Subsurfaceâ€Carbonâ€Induced Local Charge of Copper for an Onâ€Surface Displacement Reaction. Angewandte Chemie, 2021, 133, 23307.	2.0	0
10	Subsurfaceâ€Carbonâ€Induced Local Charge of Copper for an Onâ€Surface Displacement Reaction. Angewandte Chemie - International Edition, 2021, 60, 23123-23127.	13.8	6
11	Cyclic Single Atom Vertical Manipulation on a Nonmetallic Surface. Journal of Physical Chemistry Letters, 2021, 12, 11383-11390.	4.6	0
12	Voltage- and Redox State-Triggered Oxygen Adatom Conductance Switch. Journal of Physical Chemistry C, 2021, 125, 26801-26807.	3.1	2
13	Long-range ordered and atomic-scale control of graphene hybridization by photocycloaddition. Nature Chemistry, 2020, 12, 1035-1041.	13.6	41
14	Kinetics of Growth of a Covalent Assembly of Porphyrin Molecules on a Copper Surface. Journal of Physical Chemistry C, 2020, 124, 22250-22258.	3.1	1
15	Molecular recognition and homochirality preservation of guanine tetrads in the presence of melamine. Nano Research, 2020, 13, 2427-2430.	10.4	5
16	Exactly thermalized quantum dynamics of the spin-boson model coupled to a dissipative environment. Physical Review B, 2020, 101, .	3.2	4
17	Grapheneâ€Like Covalent Organic Framework with a Wide Band Gap Synthesized On Surface via Stepwise Reactions. Angewandte Chemie, 2020, 132, 16092-16096.	2.0	1
18	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

#	ARTICLE	IF	CITATIONS
19	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
20	An Endergonic Synthesis of Single Sondheimerâ€“Wong Diyne by Local Probe Chemistry. Angewandte Chemie - International Edition, 2020, 59, 10842-10847.	13.8	27
21	An Endergonic Synthesis of Single Sondheimerâ€“Wong Diyne by Local Probe Chemistry. Angewandte Chemie, 2020, 132, 10934-10939.	2.0	1
22	Generalized Langreth rules. Physical Review B, 2020, 101, .	3.2	2
23	Efficient choice of colored noise in the stochastic dynamics of open quantum systems. Physical Review E, 2020, 102, 062134.	2.1	5
24	Energy Barrier: Focus on the Essential: Extracting the Decisive Energy Barrier of a Complex Process (Adv. Mater. Interfaces 20/2019). Advanced Materials Interfaces, 2019, 6, 1970128.	3.7	0
25	Focus on the Essential: Extracting the Decisive Energy Barrier of a Complex Process. Advanced Materials Interfaces, 2019, 6, 1900795.	3.7	2
26	Externally driven molecular ratchets on a periodic potential surface: a rate equations approach. Physical Chemistry Chemical Physics, 2019, 21, 23310-23319.	2.8	1
27	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
28	Controlling the preferential motion of chiral molecular walkers on a surface. Chemical Science, 2019, 10, 5864-5874.	7.4	6
29	On-surface synthesis on a bulk insulator surface. Journal of Physics Condensed Matter, 2018, 30, 133001.	1.8	7
30	Xanthine Quartets on Au(111). Journal of the American Chemical Society, 2018, 140, 54-57.	13.7	20
31	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
32	Hydrocarbon decomposition kinetics on the Ir(111) surface. Physical Chemistry Chemical Physics, 2018, 20, 6083-6099.	2.8	6
33	Kinetic control of molecular assembly on surfaces. Communications Chemistry, 2018, 1, .	4.5	6
34	Phase-field method for epitaxial kinetics on surfaces. Journal of Chemical Physics, 2018, 149, 194107.	3.0	1
35	Formation of Hypoxanthine Tetrad by Reaction with Sodium Chloride: From Planar to Stereo. Angewandte Chemie, 2018, 130, 16247-16251.	2.0	4
36	Formation of Hypoxanthine Tetrad by Reaction with Sodium Chloride: From Planar to Stereo. Angewandte Chemie - International Edition, 2018, 57, 16015-16019.	13.8	11

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37	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
38	Driving spin-boson models from equilibrium using exact quantum dynamics. Physical Review B, 2018, 97, .	3.2	8
39	Nonadiabatic dynamics of electrons and atoms under nonequilibrium conditions. Physical Review B, 2018, 98, .	3.2	9
40	A free energy study of carbon clusters on Ir(111): Precursors to graphene growth. Journal of Chemical Physics, 2017, 146, 044702.	3.0	9
41	Mechanisms of Covalent Dimerization on a Bulk Insulating Surface. Journal of Physical Chemistry C, 2017, 121, 10053-10062.	3.1	9
42	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
43	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
44	Ethylene Dissociation on Ni₃Al(111). Journal of Physical Chemistry C, 2017, 121, 7967-7976.	3.1	2
45	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
46	Partition-free approach to open quantum systems in harmonic environments: An exact stochastic Liouville equation. Physical Review B, 2017, 95, .	3.2	14
47	Modelling a Bistable System Strongly Coupled to a Debye Bath: A Quasiclassical Approach Based on the Generalised Langevin Equation. Computational Methods in Science and Technology, 2017, 23, .	0.3	0
48	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
49	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
50	Ethylene decomposition on Ir(111): initial path to graphene formation. Physical Chemistry Chemical Physics, 2016, 18, 27897-27909.	2.8	28
51	Mathematics for Natural Scientists II. Undergraduate Lecture Notes in Physics, 2016, , .	0.1	2
52	c-number quantum generalized Langevin equation for an open system. Physical Review B, 2016, 94, .	3.2	8
53	Nonequilibrium processes from generalized Langevin equations: Realistic nanoscale systems connected to two thermal baths. Physical Review B, 2016, 93, .	3.2	14
54	Fluctuating-bias controlled electron transport in molecular junctions. Physical Review B, 2016, 93, .	3.2	14

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55	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
56	Promoting Atoms into Delocalized Long-Living Magnetically Modified State Using Atomic Force Microscopy. Nano Letters, 2016, 16, 7490-7494.	9.1	2
57	Mathematics for Natural Scientists. Undergraduate Lecture Notes in Physics, 2016, , .	0.1	2
58	Current through a multilead nanojunction in response to an arbitrary time-dependent bias. Physical Review B, 2015, 91, .	3.2	38
59	Dynamical behavior of a dangling bond dimer on a hydrogenated semiconductor: Ge(001):H. Physical Review B, 2015, 92, .	3.2	11
60	Applications of the generalized Langevin equation: Towards a realistic description of the baths. Physical Review B, 2015, 91, .	3.2	21
61	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
62	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
63	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
64	Pauliâ€™s Principle in Probe Microscopy. Advances in Atom and Single Molecule Machines, 2015, , 1-24.	0.0	1
65	Intramolecular bonds resolved on a semiconductor surface. Physical Review B, 2014, 90, .	3.2	29
66	Image formation and contrast inversion in noncontact atomic force microscopy imaging of oxidized Cu(110) surfaces. Physical Review B, 2014, 90, .	3.2	8
67	Mapping the force field of a hydrogen-bonded assembly. Nature Communications, 2014, 5, 3931.	12.8	133
68	Optimization algorithm for rate equations with an application to epitaxial graphene. Journal of Physics Condensed Matter, 2014, 26, 185008.	1.8	3
69	Generalized Langevin equation: An efficient approach to nonequilibrium molecular dynamics of open systems. Physical Review B, 2014, 89, .	3.2	54
70	Growth of epitaxial graphene: Theory and experiment. Physics Reports, 2014, 542, 195-295.	25.6	228
71	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
72	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

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73	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
74	Vertical atomic manipulation with dynamic atomic-force microscopy without tip change via a multi-step mechanism. Nature Communications, 2014, 5, 4476.	12.8	32
75	Identifying tips for intramolecular NC-AFM imaging via in situ fingerprinting. Scientific Reports, 2014, 4, 6678.	3.3	16
76	Guanine Assemblies on the Au(111) Surface: A Theoretical Study. Journal of Physical Chemistry C, 2013, 117, 5684-5692.	3.1	10
77	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
78	Construction of atomic-scale logic gates on a surface of hydrogen passivated germanium. Microelectronic Engineering, 2013, 109, 262-265.	2.4	13
79	Structural development and energy dissipation in simulated silicon apices. Beilstein Journal of Nanotechnology, 2013, 4, 941-948.	2.8	4
80	Role of orbital overlap in atomic manipulation. Physical Review B, 2012, 85, .	3.2	28
81	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
82	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
83	Complex design of dissipation signals in non-contact atomic force microscopy. Physical Chemistry Chemical Physics, 2012, 14, 16250.	2.8	11
84	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
85	Chemical tip fingerprinting in scanning probe microscopy of an oxidized Cu(110) surface. Physical Review B, 2012, 86, .	3.2	21
86	Identifying passivated dynamic force microscopy tips on H:Si(100). Applied Physics Letters, 2012, 100, .	3.3	22
87	Formation Mechanism for a Hybrid Supramolecular Network Involving Cooperative Interactions. Physical Review Letters, 2012, 108, 176103.	7.8	34
88	Homochiral Xanthine Quintet Networks Self-Assembled on Au(111) Surfaces. ACS Nano, 2011, 5, 6651-6660.	14.6	18
89	Toggling Bistable Atoms via Mechanical Switching of Bond Angle. Physical Review Letters, 2011, 106, 136101.	7.8	77
90	Architecture of PTCDA molecular structures on a reconstructed InSb(001) surface. Physical Review B, 2011, 83, .	3.2	7

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91	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
92	Ostwald ripening of binary alloy particles. Journal of Chemical Physics, 2011, 134, 024521.	3.0	15
93	Modelling components of future molecular devices. Journal of Physics Condensed Matter, 2010, 22, 084024.	1.8	3
94	Temperature control in molecular dynamic simulations of non-equilibrium processes. Journal of Physics Condensed Matter, 2010, 22, 074205.	1.8	33
95	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
96	Structure of InSb(001) surface. Journal of Physics Condensed Matter, 2010, 22, 265001.	1.8	5
97	Experimental and theoretical analysis of H-bonded supramolecular assemblies of PTCDA molecules. Physical Review B, 2010, 81, .	3.2	53
98	Structure of the indium-rich InSb(001) surface. Physical Review B, 2010, 82, .	3.2	14
99	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
100	Arrow diagram theory for non-orthogonal electronic groups: the continued fractions method. Journal of Physics Condensed Matter, 2009, 21, 474204.	1.8	0
101	Modelling the manipulation of C₆₀on the Si(001) surface performed with NC-AFM. Nanotechnology, 2009, 20, 135706.	2.6	23
102	Partitioning scheme for density functional calculations of extended systems. Journal of Chemical Physics, 2009, 130, 144104.	3.0	16
103	Prochiral Guanine Adsorption on Au(111): An Entropyâ€Stabilized Intermixed Guanineâ€Quartet Chiral Structure. Small, 2009, 5, 1952-1956.	10.0	65
104	Homopairings of the Artificial Nucleobase 1H-Benzoimidazole-4,7-dione. Journal of Physical Chemistry B, 2009, 113, 16016-16020.	2.6	0
105	H-Bonding Supramolecular Assemblies of PTCDI Molecules on the Au(111) Surface. Journal of Physical Chemistry C, 2009, 113, 21840-21848.	3.1	56
106	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
107	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
108	Multi-Scale Modelling of NC-AFM Imaging and Manipulation at Insulating Surfaces. Nanoscience and Technology, 2009, , 251-273.	1.5	0

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109	THEORETICAL MODELLING OF TIP-INDUCED MANIPULATION OF C₆₀ ON THE Si(001) SURFACE. , 2009, , .		0
110	Constrained Molecular Manipulation Mediated by Attractive and Repulsive Tipâ€“Adsorbate Forces. Small, 2008, 4, 765-769.	10.0	7
111	An Investigation into the Interactions Between Selfâ€Assembled Adenine Molecules and a Au(111) Surface. Small, 2008, 4, 1494-1500.	10.0	98
112	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
113	Melamine Structures on the Au(111) Surface. Journal of Physical Chemistry C, 2008, 112, 11476-11480.	3.1	122
114	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
115	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
116	Comparative Theoretical Study of O- and S-Containing Hydrogen-Bonded Supramolecular Structures. Journal of Physical Chemistry C, 2008, 112, 17340-17350.	3.1	8
117	Understanding the disorder of the DNA base cytosine on the Au(111) surface. Journal of Chemical Physics, 2008, 129, 184707.	3.0	57
118	Elementary Structural Motifs in a Random Network of Cytosine Adsorbed on a Gold(111) Surface. Science, 2008, 319, 312-315.	12.6	157
119	Theoretical modelling of tip effects in the pushing manipulation of C₆₀on the Si(001) surface. Nanotechnology, 2008, 19, 235702.	2.6	14
120	Theoretical study of melamine superstructures and their interaction with the Au(111) surface. Nanotechnology, 2008, 19, 465704.	2.6	39
121	Generalized Langevin equation for solids. I. Rigorous derivation and main properties. Physical Review B, 2008, 78, .	3.2	62
122	Vertical manipulation of a molecule with chemical forces. Physical Review B, 2008, 77, .	3.2	8
123	Generalized Langevin equation for solids. II. Stochastic boundary conditions for nonequilibrium molecular dynamics simulations. Physical Review B, 2008, 78, .	3.2	53
124	Dihydride dimer structures on the Si(100):H surface studied by low-temperature scanning tunneling microscopy. Physical Review B, 2008, 78, .	3.2	25
125	Interpretation of atomic friction experiments based on atomistic simulations. Journal of Vacuum Science & Technology B, 2007, 25, 1547.	1.3	13
126	A comparison of dynamic atomic force microscope set-ups for performing atomic scale manipulation experiments. Nanotechnology, 2007, 18, 345503.	2.6	5

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127	Is atomic-scale dissipation in NC-AFM real? Investigation using virtual atomic force microscopy. Nanotechnology, 2007, 18, 084017.	2.6	19
128	Nonequilibrium statistical mechanics of classical nuclei interacting with the quantum electron gas. Physical Review B, 2007, 76, .	3.2	8
129	Simulating system dynamics with arbitrary time step. Physical Review B, 2007, 75, .	3.2	13
130	Treating periodic systems using embedding: Adams-Gilbert approach. Physical Review B, 2007, 76, .	3.2	17
131	Controlled Manipulation of Atoms in Insulating Surfaces with the Virtual Atomic Force Microscope. Physical Review Letters, 2007, 98, 028101.	7.8	39
132	Dynamical processes at oxide surfaces studied with the virtual atomic force microscope. Physical Review B, 2007, 76, .	3.2	26
133	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
134	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
135	Coexistence of Homochiral and Heterochiral Adenine Domains at the Liquid/Solid Interface. Journal of Physical Chemistry B, 2007, 111, 12048-12052.	2.6	48
136	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
137	Theory of Adsorption and Manipulation of C60 on the Si(001) Surface. Nanoscience and Technology, 2007, , 601-618.	1.5	0
138	Mechanisms of atomic scale dissipation at close approach in dynamic atomic force microscopy. Nanoscience and Technology, 2007, , 373-391.	1.5	0
139	Planar nucleic acid base super-structures. Journal of Materials Chemistry, 2006, 16, 1894.	6.7	52
140	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
141	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
142	Arrow diagram approach to nonorthogonal electron group functions in extended systems. Journal of Physics Condensed Matter, 2006, 18, 295-313.	1.8	3
143	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
144	Modelling atomic scale manipulation with the non-contact atomic force microscope. Nanotechnology, 2006, 17, 5866-5874.	2.6	26

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145	Origin ofp(2Ã—1)Phase on Si(001) by Noncontact Atomic Force Microscopy at 5ÂK. Physical Review Letters, 2006, 96, 106104.	7.8	52
146	Manipulation ofC60on theSi(001)surface: Experiment and theory. Physical Review B, 2006, 74, .	3.2	19
147	Experimental and theoretical identification of adenine monolayers on Ag-terminated Si(111). Physical Review B, 2006, 73, .	3.2	46
148	Probing theSi(001)surface with a Si tip: Anab initiostudy. Physical Review B, 2006, 73, .	3.2	38
149	An ab initio study of C60 adsorption on the Si(001) surface. Surface Science, 2005, 591, 45-55.	1.9	60
150	Hexagonal adenine networks constructed from their homopairings. Surface Science, 2005, 589, 139-152.	1.9	30
151	Molecular dynamics simulations of atomic scale processes at close approach in non-contact atomic force microscopy. Nanotechnology, 2005, 16, S79-S84.	2.6	30
152	Bond Breaking Coupled with Translation in Rolling of Covalently Bound Molecules. Physical Review Letters, 2005, 94, 146104.	7.8	85
153	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
154	Homopairing Possibilities of the DNA Base Adenine. Journal of Physical Chemistry B, 2005, 109, 11933-11939.	2.6	67
155	Physical dissipation mechanisms in non-contact atomic force microscopy. Nanotechnology, 2004, 15, S44-S48.	2.6	25
156	Strongly localized molecular orbitals for Â-quartz. Journal of Physics Condensed Matter, 2004, 16, 7233-7246.	1.8	4
157	The interstitial CiOi defect in bulk Si and Si1ÂxGex. Journal of Physics Condensed Matter, 2004, 16, 8545-8555.	1.8	5
158	Electron density of periodic systems derived from non-orthogonal localized orbitals. Journal of Physics Condensed Matter, 2004, 16, 2575-2584.	1.8	9
159	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
160	General Theory of Microscopic Dynamical Response in Surface Probe Microscopy: From Imaging to Dissipation. Physical Review Letters, 2004, 93, 236102.	7.8	130
161	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
162	Comparison of localization procedures for applications in crystal embedding. Physical Review B, 2004, 70, .	3.2	12

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163	Adsorption of C60on the Si(001) surface calculated within the generalized gradient approximation. Nanotechnology, 2004, 15, S1-S4.	2.6	26
164	Interstitial oxygen in Si andSi1â^'xGex. Physical Review B, 2004, 69, .	3.2	25
165	Sublattice Identification in Scanning Force Microscopy on Alkali Halide Surfaces. Physical Review Letters, 2004, 92, 146103.	7.8	102
166	Quantum Theory of the Solid State: An Introduction. , 2004, , .		45
167	Tip models and force definitions in molecular dynamics simulations of scanning force microscopy. Surface Science, 2003, 540, 497-503.	1.9	19
168	Exact calculation of the tip friction within the harmonic model. Applied Surface Science, 2003, 210, 27-31.	6.1	8
169	Non-equilibrium dynamics of a classical tip interacting with a quantum surface. Journal of Physics Condensed Matter, 2002, 14, 7123-7133.	1.8	7
170	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
171	Atomic corrugation in nc-AFM of alkali halides. Applied Surface Science, 2002, 188, 232-237.	6.1	32
172	Quantum theory of energy dissipation in non-contact atomic force microscopy in Markovian approximation. Surface Science, 2002, 521, 117-128.	1.9	8
173	Theory of Energy Dissipation into Surface Vibrations. Nanoscience and Technology, 2002, , 371-394.	1.5	9
174	A simple non-equilibrium theory of non-contact dissipation force microscopy. Journal of Physics Condensed Matter, 2001, 13, 945-958.	1.8	24
175	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
176	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
177	Application of the group function theory to infinite systems. International Journal of Quantum Chemistry, 2000, 76, 511-534.	2.0	10
178	Derivation of atomistic models for lattices consisting of weakly overlapping structural elements. International Journal of Quantum Chemistry, 2000, 78, 306-330.	2.0	11
179	Atomically resolved edges and kinks of NaCl islands on Cu(111): Experiment and theory. Physical Review B, 2000, 62, 2074-2084.	3.2	213
180	Structure and Spectroscopy of Surface Defects from Scanning Force Microscopy: Theoretical Predictions. Physical Review Letters, 2000, 85, 3846-3849.	7.8	12

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