Adalberto Fazzio

List of Publications by Year
in descending order

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311 papers	10,361 citations	34016 52 h-index	46693 89 g-index
313 all docs	313 docs citations	313 times ranked	9636 citing authors

#	Article	IF	Citations
1	Machine Learning of Microscopic Ingredients for Graphene Oxide/Cellulose Interaction. Langmuir, 2022, 38, 1124-1130.	1.6	8
2	Daphnia magna and mixture toxicity with nanomaterials â€“ Current status and perspectives in data-driven risk prediction. Nano Today, 2022, 43, 101430.	6.2	20
3	High-throughput inverse design and Bayesian optimization of functionalities: spin splitting in two-dimensional compounds. Scientific Data, 2022, 9, 195.	2.4	2
4	Role of Functional Thiolated Molecules on the Enhanced Electronic Transport of Interconnected MoS₂ Nanostructures. Journal of Physical Chemistry C, 2022, 126, 12159-12167.	1.5	0
5	Distilling small volumes of crude oil. Fuel, 2021, 285, 119072.	3.4	8
6	Disorder effects of vacancies on the electronic transport properties of realistic topological insulator nanoribbons: The case of bismuthene. Physical Review Materials, 2021, 5, .	0.9	14
7	Bandgap evolution in nanographene assemblies. Physical Chemistry Chemical Physics, 2021, 23, 11501-11506.	1.3	1
8	Structural and electronic properties of realistic two-dimensional amorphous topological insulators. 2D Materials, 2021, 8, 025032.	2.0	16
9	Pair Distribution Function Obtained from Electron Diffraction: An Advanced Real-Space Structural Characterization Tool. Matter, 2021, 4, 441-460.	5.0	29
10	Disassembly of TEMPO-Oxidized Cellulose Fibers: Intersheet and Interchain Interactions in the Isolation of Nanofibers and Unitary Chains. Journal of Physical Chemistry B, 2021, 125, 3717-3724.	1.2	6
11	Discovery of higher-order topological insulators using the spin Hall conductivity as a topology signature. Npj Computational Materials, 2021, 7, .	3.5	15
12	Unveiling the dopant segregation effect at hematite interfaces. Applied Physics Letters, 2021, 118, .	1.5	13
13	Conformational analysis of tannic acid: Environment effects in electronic and reactivity properties. Journal of Chemical Physics, 2021, 154, 224102.	1.2	3
14	Recent Advances in Immunosafety and Nanoinformatics of Two-Dimensional Materials Applied to Nano-imaging. Frontiers in Immunology, 2021, 12, 689519.	2.2	5
15	Roomâ€Temperature Negative Differential Resistance in Surfaceâ€Supported Metalâ€Organic Framework Vertical Heterojunctions. Small, 2021, 17, e2101475.	5.2	6
16	Machine learning for materials discovery: Two-dimensional topological insulators. Applied Physics Reviews, 2021, 8, .	5.5	34
17	Emergent quasiparticles in Euclidean tilings. Nanoscale, 2021, 13, 5270-5274.	2.8	4
18	At the Verge of Topology: Vacancy-Driven Quantum Spin Hall in Trivial Insulators. Nano Letters, 2021, 21, 9398-9402.	4.5	5

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19	Amorphous <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mrow><mml:mi>Bi</mml:mi></mml:mrow><mml:mn>2</mml:mn> structural, electronic, and topological nature from first principles. Physical Review B, 2021, 104, .		
20	Exploring Two-Dimensional Materials Thermodynamic Stability via Machine Learning. ACS Applied Materials & Interfaces, 2020, 12, 20149-20157.	4.0	80
21	Ab Initio Simulations and Materials Chemistry in the Age of Big Data. Journal of Chemical Information and Modeling, 2020, 60, 452-459.	2.5	28
22	Ambipolar Resistive Switching in an Ultrathin Surface-Supported Metalâ€“Organic Framework Vertical Heterojunction. Nano Letters, 2020, 20, 1080-1088.	4.5	53
23	Ordinary microfluidic electrodes combined with bulk nanoprobe produce multidimensional electric double-layer capacitances towards metal ion recognition. Sensors and Actuators B: Chemical, 2020, 305, 127482.	4.0	16
24	The Rashba Scale: Emergence of Band Anti-crossing as a Design Principle for Materials with Large Rashba Coefficient. Matter, 2020, 3, 145-165.	5.0	21
25	Dual topological insulator device with disorder robustness. Physical Review B, 2020, 102, .	1.1	11
26	Inverse design of compounds that have simultaneously ferroelectric and Rashba cofunctionality. Physical Review B, 2020, 102, .	1.1	20
27	Simulations of X-ray absorption spectroscopy and energetic conformation of N-heterocyclic carbenes on Au(111). Physical Chemistry Chemical Physics, 2020, 22, 21504-21511.	1.3	6
28	Converging Multidimensional Sensor and Machine Learning Toward High-Throughput and Biorecognition Element-Free Multidetermination of Extracellular Vesicle Biomarkers. ACS Sensors, 2020, 5, 1864-1871.	4.0	20
29	Pair Distribution Function from Electron Diffraction in Cryogenic Electron Microscopy: Revealing Glassy Water Structure. Journal of Physical Chemistry Letters, 2020, 11, 1564-1569.	2.1	16
30	The 2021 quantum materials roadmap. JPhys Materials, 2020, 3, 042006.	1.8	111
31	Jacutingaite-family: A class of topological materials. Physical Review B, 2020, 102, .	1.1	13
32	Toward Realistic Amorphous Topological Insulators. Nano Letters, 2019, 19, 8941-8946.	4.5	44
33	Zeeman-type spin splitting in nonmagnetic three-dimensional compounds. Npj Quantum Materials, 2019, 4, .	1.8	23
34	Metal Chalcogenides Janus Monolayers for Efficient Hydrogen Generation by Photocatalytic Water Splitting. ACS Applied Nano Materials, 2019, 2, 890-897.	2.4	93
35	Spin-Polarization Control Driven by a Rashba-Type Effect Breaking the Mirror Symmetry in Two-Dimensional Dual Topological Insulators. Physical Review Letters, 2019, 122, 036401.	2.9	25
36	Theoretical and Experimental Investigation of 2D Hematite. Journal of Physical Chemistry C, 2019, 123, 16359-16365.	1.5	17

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37	Electronic transport properties of MoS2 nanoribbons embedded in butadiene solvent. Physical Chemistry Chemical Physics, 2019, 21, 11359-11366.	1.3	11
38	Decreasing Nanocrystal Structural Disorder by Ligand Exchange: An Experimental and Theoretical Analysis. Journal of Physical Chemistry Letters, 2019, 10, 1471-1476.	2.1	19
39	From DFT to machine learning: recent approaches to materials scienceâ€“a review. JPhys Materials, 2019, 2, 032001.	1.8	385
40	The role played by the molecular geometry on the electronic transport through nanometric organic films. Physical Chemistry Chemical Physics, 2019, 21, 24584-24591.	1.3	3
41	Structural evolution and the role of native defects in subnanometer MoS nanowires. Physical Review B, 2019, 100, .	1.1	7
42	Oxidation of Ni 13 clusters. International Journal of Quantum Chemistry, 2019, 119, e25874.	1.0	4
43	Semiclassical transport properties of IrGa₃: a promising thermoelectric material. Journal of Physics Condensed Matter, 2018, 30, 085701.	0.7	7
44	Nanoporous ZnO: Structural and electronic study under biaxial strain. Computational Materials Science, 2018, 149, 91-97.	1.4	0
45	Controlling Topological States in Topological/Normal Insulator Heterostructures. ACS Omega, 2018, 3, 15900-15906.	1.6	10
46	Band gap tuning of layered III-Te materials. Journal of Applied Physics, 2018, 124, .	1.1	7
47	Tight-binding model for the band dispersion in rhombohedral topological insulators over the whole Brillouin zone. Physical Review B, 2018, 98, .	1.1	10
48	Layer-dependent band alignment of few layers of blue phosphorus and their van der Waals heterostructures with graphene. Physical Review B, 2018, 97, .	1.1	45
49	Silicene-Based FET for Logical Technology. IEEE Electron Device Letters, 2018, 39, 1258-1261.	2.2	10
50	Oxidation of free-standing and supported borophene. 2D Materials, 2017, 4, 025025.	2.0	31
51	Stacking-dependent transport properties in few-layers graphene. Solid State Communications, 2017, 250, 70-74.	0.9	10
52	Adsorption of 3d, 4d, and 5dtransition metal atoms onÎ²₁₂â€”Borophene. Journal of Physics Condensed Matter, 2017, 29, 305302.	0.7	16
53	Tuning the p-type Schottky barrier in 2D metal/semiconductor interface:boron-sheet on MoSe2, and WSe2. Journal of Physics Condensed Matter, 2017, 29, 405002.	0.7	3
54	Nanodots of transition metal dichalcogenides embedded in MoS2 and MoSe2: first-principles calculations. Physical Chemistry Chemical Physics, 2017, 19, 26240-26247.	1.3	0

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55	Dynamic covalent bond from first principles: Diarylbibenzofuranone structural, electronic, and oxidation studies. Journal of Computational Chemistry, 2017, 38, 2675-2679.	1.5	3
56	Novel III-Teâ€“graphene van der Waals heterojunctions for optoelectronic devices. RSC Advances, 2017, 7, 32383-32390.	1.7	8
57	Two-dimensional van der Waals p-n junction of InSe/phosphorene. Physical Review B, 2017, 95, .	1.1	68
58	Topological states of nanoscale Bi2Se3 interfaced with AlN. Applied Physics Letters, 2016, 109, 131601.	1.5	5
59	Directional dependence of the electronic and transport properties of 2D borophene and borophane. Physical Chemistry Chemical Physics, 2016, 18, 25491-25496.	1.3	92
60	Fully and partially iodinated germanane as a platform for the observation of the quantum spin Hall effect. Physical Review B, 2016, 93, .	1.1	18
61	Unconventional spin texture in a noncentrosymmetric quantum spin Hall insulator. Physical Review B, 2016, 94, .	1.1	22
62	Substrate-supported large-band-gap quantum spin Hall insulator based on III-V bismuth layers. Physical Review B, 2016, 94, .	1.1	4
63	A new class of large band gap quantum spin hall insulators: 2D fluorinated group-IV binary compounds. Scientific Reports, 2016, 6, 26123.	1.6	17
64	On the nature of the solvated electron in ice I_h. Physical Chemistry Chemical Physics, 2016, 18, 4652-4658.	1.3	6
65	Topological phase transitions of (BixSb1â^'x)2Se3 alloys by density functional theory. Journal of Physics Condensed Matter, 2015, 27, 255501.	0.7	10
66	Valley Hall effect in silicene and hydrogenated silicene ruled by grain boundaries: Anab initioinvestigation. Physical Review B, 2015, 91, .	1.1	11
67	van der Waals Heterostructure of Phosphorene and Graphene: Tuning the Schottky Barrier and Doping by Electrostatic Gating. Physical Review Letters, 2015, 114, 066803.	2.9	445
68	Switching a Normal Insulator into a Topological Insulator via Electric Field with Application to Phosphorene. Nano Letters, 2015, 15, 1222-1228.	4.5	406
69	Vertical twinning of the Dirac cone at the interface between topological insulators and semiconductors. Nature Communications, 2015, 6, 7630.	5.8	26
70	Tuning the thermoelectric properties of a single-molecule junction by mechanical stretching. Physical Chemistry Chemical Physics, 2015, 17, 5386-5392.	1.3	13
71	First-principles study of HgTe/CdTe heterostructures under perturbations preserving time-reversal symmetry. Physical Review B, 2014, 90, .	1.1	14
72	Spin caloritronics in graphene with Mn. Applied Physics Letters, 2014, 104, .	1.5	18

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73	Topological phases in triangular lattices of Ru adsorbed on graphene:Ab initiocalculations. Physical Review B, 2014, 89, .	1.1	25
74	Size- effect induced high thermoelectric figure of merit in PbSe and PbTe nanowires. Physical Chemistry Chemical Physics, 2014, 16, 8114-8118.	1.3	15
75	Directional Control of the Electronic and Transport Properties of Graphynes. Journal of Physical Chemistry C, 2014, 118, 18793-18798.	1.5	18
76	Quantum spin Hall effect on germanene nanorod embedded in completely hydrogenated germanene. Physical Review B, 2014, 89, .	1.1	57
77	Graphene on amorphous HfO2surface: Anab initioinvestigation. Physical Review B, 2013, 87, .	1.1	12
78	Graphene nanoribbon intercalated with hexagonal boron nitride: Electronic transport properties from ab initio calculations. Solid State Communications, 2013, 173, 24-29.	0.9	10
79	Topological insulator Bi<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mrow /><mml:mn>2</mml:mn></mml:msub></mml:math>Se<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>(111) surface doped with transition metals: Anab initioinvestigation. Physical Review B, 2013, 88, .	1.1	52
80	Electronic transport in patterned graphene nanoroads. Nanotechnology, 2013, 24, 495201.	1.3	10
81	Quantum spin Hall effect in a disordered hexagonal Si<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mrow /><mml:mi>x</mml:mi></mml:msub></mml:math>Ge<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mrow /><mml:mrow><mml:mn>1</mml:mn><mml:mo>â”</mml:mo><mml:mi>x</mml:mi></mml:mrow></mml:msub></mml:math>alloy. Physical Review B, 2013, 88, .	1.1	24
82	Topological states ruled by stacking faults in Bi2Se3 and Bi2Te3. Journal of Applied Physics, 2013, 113, 023705.	1.1	21
83	Confinement effects and why carbon nanotube bundles can work as gas sensors. Nanoscale, 2013, 5, 2798.	2.8	25
84	First-principles study of group III impurity doped PbSe: Bulk and nanowire. Physical Review B, 2013, 87, .	1.1	8
85	Carrier-mediated magnetism in transition metal doped Bi2Se3 topological insulator. Journal of Physics Condensed Matter, 2013, 25, 445003.	0.7	5
86	Interfaces between buckling phases in silicene:Ab initiodensity functional theory calculations. Physical Review B, 2013, 88, .	1.1	11
87	ConsideraÃ§Ãµes sobre o Programa Brasileiro de Nanotecnologia. CiÃªncia E Cultura, 2013, 65, 23-27.	0.5	2
88	Publisher's Note: Quantum confinement and spin-orbit interactions in PbSe and PbTe nanowires: First-principles calculation [Phys. Rev. B84, 245324 (2011)]. Physical Review B, 2012, 86, .	1.1	0
89	Tuning Low-Spin to High-Spin Mn Pairs in 2-D ZnO by Injecting Holes. IEEE Nanotechnology Magazine, 2012, 11, 71-76.	1.1	1
90	Bilayer graphene on h-BN substrate: investigating the breakdown voltage and tuning the bandgap by electric field. Journal of Physics Condensed Matter, 2012, 24, 075301.	0.7	22

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91	Light emission and current rectification in a molecular device: Experiment and theory. Journal of Applied Physics, 2012, 112, 113108.	1.1	0
92	Ab-initio calculations for a realistic sensor: A study of CO sensors based on nitrogen-rich carbon nanotubes. AIP Advances, 2012, 2, .	0.6	10
93	Adatoms in graphene as a source of current polarization: Role of the local magnetic moment. Physical Review B, 2011, 84, .	1.1	27
94	Ab Initio Calculations of Structural Evolution and Conductance of Benzene-1,4-dithiol on Gold Leads. ACS Nano, 2011, 5, 795-804.	7.3	89
95	Piezomagnetic behavior of Co-doped ZnO nanoribbons. Physical Review B, 2011, 84, .	1.1	7
96	Doping of graphene adsorbed on the a-SiO2 surface. Applied Physics Letters, 2011, 99, 163108.	1.5	46
97	Mn dimers on graphene nanoribbons: An ab initio study. Journal of Applied Physics, 2011, 109, 053715.	1.1	15
98	Quantum confinement and spin-orbit interactions in PbSe and PbTe nanowires: First-principles calculation. Physical Review B, 2011, 84, .	1.1	10
99	Bilayer graphene dual-gate nanodevice: Anab initiosimulation. Physical Review B, 2011, 84, .	1.1	36
100	Spin filtering and disorder-induced magnetoresistance in carbon nanotubes:Ab initiocalculations. Physical Review B, 2011, 84, .	1.1	14
101	Spin texture and magnetic anisotropy of Co impurities in Bi<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mrow /><mml:mn>2</mml:mn></mml:msub></mml:math>Se<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>topological insulators. Physical Review B, 2011, 84, .	1.1	47
102	Electronic transport properties of ascorbic acid and nicotinamide adsorbed on single-walled carbon nanotubes. Chemical Physics Letters, 2011, 506, 233-238.	1.2	13
103	IxV curves of boron and nitrogen doping zigzag graphene nanoribbons. International Journal of Quantum Chemistry, 2011, 111, 1379-1386.	1.0	17
104	Energetics and stability of vacancies in carbon nanotubes. Solid State Communications, 2011, 151, 482-486.	0.9	42
105	Mn-doped cubic BN as an atomiclike memory device: A density functional study. Physical Review B, 2010, 81, .	1.1	2
106	Splitting of the zero-energy edge states in bilayer graphene. Physical Review B, 2010, 81, .	1.1	14
107	Disorder-based graphene spintronics. Nanotechnology, 2010, 21, 345202.	1.3	30
108	Origin of FM Ordering in Pristine Micro- and Nanostructured ZnO. Nano Letters, 2010, 10, 1383-1386.	4.5	98

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109	Ferromagnetic coupling in a Co-doped graphenelike ZnO sheet. Physical Review B, 2010, 81, .	1.1	62
110	Mimicking nanoribbon behavior using a graphene layer on SiC. Physical Review B, 2010, 82, .	1.1	8
111	Surface and Quantum Confinement Effects in ZnO Nanocrystals. Journal of Physical Chemistry C, 2010, 114, 18293-18297.	1.5	53
112	Formation of atomic carbon chains from graphene nanoribbons. Physical Review B, 2010, 81, .	1.1	54
113	Realistic calculations of carbon-based disordered systems. Journal Physics D: Applied Physics, 2010, 43, 374002.	1.3	19
114	Organic molecule assembled between carbon nanotubes: A highly efficient switch device. Physical Review B, 2009, 79, .	1.1	36
115	MS-XÎ±: Treatment for native defects in GaSb. International Journal of Quantum Chemistry, 2009, 20, 457-457.	1.0	0
116	Native defects and transition metal impurities at interstitial sites in gaas. International Journal of Quantum Chemistry, 2009, 36, 677-685.	1.0	0
117	Surface magnetization in non-doped ZnO nanostructures. Applied Physics Letters, 2009, 94, .	1.5	74
118	Electronic, structural, and transport properties of Ni-doped graphene nanoribbons. Physical Review B, 2009, 79, .	1.1	143
119	Effects of Side-Chain and Electron Exchange Correlation on the Band Structure of Perylene Diimide Liquid Crystals: A Density Functional Study. Journal of Physical Chemistry B, 2009, 113, 5376-5380.	1.2	12
120	Edge effects in bilayer graphene nanoribbons:Ab initiototal-energy density functional theory calculations. Physical Review B, 2009, 79, .	1.1	58
121	Barrier-free substitutional doping of graphene sheets with boron atoms:Ab initiocalculations. Physical Review B, 2009, 79, .	1.1	63
122	Theoretical investigation of Hf and Zr defects in c-Ge. Journal of Physics Condensed Matter, 2009, 21, 012206.	0.7	0
123	Quantum confinement effects on Mn-doped InAs nanocrystals: A first-principles study. Physical Review B, 2008, 78, .	1.1	18
124	Hydrogen adsorption on boron doped graphene: anab initiostudy. Nanotechnology, 2008, 19, 155708.	1.3	86
125	First-principles study of the adsorption of atomic and molecular hydrogen on<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:mi mathvariant="normal">B</mml:mi><mml:msub><mml:mi mathvariant="normal">C</mml:mi><mml:mn>2</mml:mn></mml:msub><mml:mi mathvariant="normal">N</mml:mi></mml:mrow></mml:math>nanotubes. Physical Review B, 2008, 77, .	1.1	30
126	Ïƒ- and Ï€-Defects at Graphene Nanoribbon Edges: Building Spin Filters. Nano Letters, 2008, 8, 2293-2298.	4.5	101

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127	Confinement and Surface Effects in B and P Doping of Silicon Nanowires. Nano Letters, 2008, 8, 1866-1871.	4.5	53
128	Electronic and Magnetic Properties of Ti and Fe on Graphene. Journal of Physical Chemistry C, 2008, 112, 9163-9167.	1.5	91
129	Ab Initio Study of SO₂ Molecules Interacting with Pristine and Transition Metal Covered Fullerenes as a Possible Route for Nanofilters. Journal of Physical Chemistry C, 2008, 112, 6677-6680.	1.5	5
130	Symmetry Controlled Spin Polarized Conductance in Au Nanowires. Journal of the American Chemical Society, 2008, 130, 9897-9903.	6.6	20
131	Designing Real Nanotube-Based Gas Sensors. Physical Review Letters, 2008, 100, 176803.	2.9	102
132	AmorphousHfO2andHf1âˆ'xSixOvia a melt-and-quench scheme usingab initiomolecular dynamics. Physical Review B, 2008, 77, .	1.1	46
133	Transport properties of single vacancies in nanotubes. Physical Review B, 2008, 77, .	1.1	35
134	Temperature and Quantum Effects in the Stability of Pure and Doped Gold Nanowires. Physical Review Letters, 2008, 100, 056104.	2.9	30
135	Simple implementation of complex functionals: Scaled self-consistency. Journal of Chemical Physics, 2007, 126, 144107.	1.2	8
136	Theoretical investigations of Ge nanowires grown along the [110] and [111] directions. Nanotechnology, 2007, 18, 295706.	1.3	31
137	Theoretical investigation of a Mn-dopedSiâˆ•Geheterostructure. Physical Review B, 2007, 75, .	1.1	9
138	Hf defects incâˆ'Siand their importance for theHfO2âˆ•Siinterface: Density-functional calculations. Physical Review B, 2007, 75, .	1.1	4
139	EL2-like defects in InP nanowires: Anab initiototal energy investigation. Physical Review B, 2007, 75, .	1.1	6
140	Structural, electronic, and magnetic properties of Mn-doped Ge nanowires byab initiocalculations. Physical Review B, 2007, 75, .	1.1	16
141	Short linear atomic chains in copper nanowires. Nanotechnology, 2007, 18, 145701.	1.3	33
142	Divacancies in Graphene and Carbon Nanotubes. Nano Letters, 2007, 7, 2459-2462.	4.5	175
143	Si Nanowires as Sensors:Â Choosing the Right Surface. Nano Letters, 2007, 7, 1172-1177.	4.5	40
144	Electronic and Transport Properties of Boron-Doped Graphene Nanoribbons. Physical Review Letters, 2007, 98, 196803.	2.9	540

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145	Adsorption of CO and NO molecules on carbon doped boron nitride nanotubes. Solid State Communications, 2007, 142, 49-53.	0.9	112
146	First principles study of titanium-coated carbon nanotubes as sensors for carbon monoxide molecules. Surface Science, 2007, 601, 4102-4104.	0.8	23
147	Ab initio study of 2,3,7,8-tetrachlorinated dibenzo-p-dioxin adsorption on single wall carbon nanotubes. Chemical Physics Letters, 2007, 437, 79-82.	1.2	41
148	Ab initio study of pristine and Si-doped capped carbon nanotubes interacting with nimesulide molecules. Chemical Physics Letters, 2007, 439, 348-353.	1.2	39
149	Oxygen Clamps in Gold Nanowires. Physical Review Letters, 2006, 96, 016104.	2.9	64
150	Hydrogen Adsorption on Carbon-Doped Boron Nitride Nanotube. Journal of Physical Chemistry B, 2006, 110, 21184-21188.	1.2	105
151	C59Si on the Monohydride Si(100):Hâ˜(2 Ã— 1) Surface. Journal of Physical Chemistry B, 2006, 110, 10849-10854.	1.2	10
152	Adsorption of Benzene-1,4-dithiol on the Au(111) Surface and Its Possible Role in Molecular Conductance. Journal of the American Chemical Society, 2006, 128, 8996-8997.	6.6	66
153	First principles calculations of as impurities in the presence of a 90Âº partial dislocation in Si. Brazilian Journal of Physics, 2006, 36, 261-263.	0.7	6
154	Effects of disorder on the exchange coupling in (Ga,Mn)As diluted magnetic semiconductors. Brazilian Journal of Physics, 2006, 36, 813-816.	0.7	1
155	Density functional theory method for non-equilibrium charge transport calculations: TRANSAMPA. Brazilian Journal of Physics, 2006, 36, 799-807.	0.7	51
156	Phenomenological band structure model of magnetic coupling in semiconductors. Solid State Communications, 2006, 138, 353-358.	0.9	134
157	Silicon adsorption in defective carbon nanotubes: a first principles study. Nanotechnology, 2006, 17, 4088-4091.	1.3	4
158	Gold nanowires and the effect of impurities. Nanoscale Research Letters, 2006, 1, 91-98.	3.1	17
159	Titanium monomers and wires adsorbed on carbon nanotubes: a first principles study. Nanotechnology, 2006, 17, 1154-1159.	1.3	22
160	Orientational Defects in Ice Ih: An Interpretation of Electrical Conductivity Measurements. Physical Review Letters, 2006, 96, 075501.	2.9	35
161	Structure and Energetics of Molecular Point Defects in Icelh. Physical Review Letters, 2006, 97, 155501.	2.9	22
162	Electronic and magnetic properties of Mn-doped InP nanowires from first principles. Physical Review B, 2006, 73, .	1.1	30

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163	Carbon nanotube adsorbed on hydrogenated Si(001) surfaces. Applied Surface Science, 2005, 244, 124-128.	3.1	7
164	Computer simulations in the study of gold nanowires: the effect of impurities. Applied Physics A: Materials Science and Processing, 2005, 81, 1551-1558.	1.1	15
165	Electronic and structural properties of C59Si on the monohydride Si(100) surface. International Journal of Quantum Chemistry, 2005, 103, 557-561.	1.0	3
166	Comment on â€œContaminants in Suspended Gold Chains: AnAbÂInitioMolecular Dynamics Studyâ€• Physical Review Letters, 2005, 95, 169601; author reply 169602.	2.9	12
167	Disorder and the effectiveMnâˆ’Mnexchange interaction inGa1âˆ’xMnxAsdiluted magnetic semiconductors. Physical Review B, 2005, 72, .	1.1	13
168	Oxygen-induced atomic desorptions in oxynitrides: Density functional calculations. Physical Review B, 2005, 72, .	1.1	5
169	Substrate-dependent electronic properties of an armchair carbon nanotube adsorbed on Hâˆ•Si(001). Applied Physics Letters, 2005, 86, 213111.	1.5	34
170	Formation energy of native defects in BN nanotubes: anab initiostudy. Nanotechnology, 2005, 16, 827-831.	1.3	74
171	Stability and electronic confinement of free-standingInPnanowires:Ab initiocalculations. Physical Review B, 2005, 72, .	1.1	35
172	Bundling up Carbon Nanotubes through Wigner Defects. Nano Letters, 2005, 5, 1045-1049.	4.5	32
173	Vacancy Formation Process in Carbon Nanotubes:Â First-Principles Approach. Nano Letters, 2005, 5, 197-200.	4.5	76
174	Anab initiostudy of manganese atoms and wires interacting with carbon nanotubes. Journal of Physics Condensed Matter, 2004, 16, 3647-3661.	0.7	16
175	Stabilization of substitutional Mn in silicon-based semiconductors. Physical Review B, 2004, 70, .	1.1	38
176	Initial stages of Ge and Si growth nearSBmonoatomic steps on Si(100). Physical Review B, 2004, 70, .	1.1	3
177	Theoretical study of the formation, evolution, and breaking of gold nanowires. Physical Review B, 2004, 69, .	1.1	110
178	Carbon inSixGe1âˆ’x:Anab initioinvestigation. Physical Review B, 2004, 69, .	1.1	8
179	Diffusion-reaction mechanisms of nitriding species inSiO2. Physical Review B, 2004, 70, .	1.1	20
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