Adalberto Fazzio

List of Publications by Year in Descending Order

305 papers	8,752 citations	48 h-index	83 g-index
313 ext. papers	9,520 ext. citations	4 avg, IF	6.28 L-index

#	Paper	IF	Citations
305	Daphnia magna and mixture toxicity with nanomaterials Current status and perspectives in data-driven risk prediction. *Nano Today*, **2022**, 43, 101430	17.9	2
304	High-throughput inverse design and Bayesian optimization of functionalities: spin splitting in two-dimensional compounds.. *Scientific Data*, **2022**, 9, 195	8.2	
303	At the Verge of Topology: Vacancy-Driven Quantum Spin Hall in Trivial Insulators. *Nano Letters*, **2021**, 21, 9398-9402	11.5	0
302	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	3.4	0
301	Discovery of higher-order topological insulators using the spin Hall conductivity as a topology signature. *Npj Computational Materials*, **2021**, 7,	10.9	2
300	Unveiling the dopant segregation effect at hematite interfaces. *Applied Physics Letters*, **2021**, 118, 201602	3.4	4
299	Conformational analysis of tannic acid: Environment effects in electronic and reactivity properties. *Journal of Chemical Physics*, **2021**, 154, 224102	3.9	0
298	Recent Advances in Immunosafety and Nanoinformatics of Two-Dimensional Materials Applied to Nano-imaging. *Frontiers in Immunology*, **2021**, 12, 689519	8.4	1
297	Room-Temperature Negative Differential Resistance in Surface-Supported Metal-Organic Framework Vertical Heterojunctions. *Small*, **2021**, 17, e2101475	11	3
296	Distilling small volumes of crude oil. *Fuel*, **2021**, 285, 119072	7.1	2
295	Disorder effects of vacancies on the electronic transport properties of realistic topological insulator nanoribbons: The case of bismuthene. *Physical Review Materials*, **2021**, 5,	3.2	4
294	Bandgap evolution in nanographene assemblies. *Physical Chemistry Chemical Physics*, **2021**, 23, 11501-11506	3.6	1
293	Structural and electronic properties of realistic two-dimensional amorphous topological insulators. *2D Materials*, **2021**, 8, 025032	5.9	6
292	Pair Distribution Function Obtained from Electron Diffraction: An Advanced Real-Space Structural Characterization Tool. *Matter*, **2021**, 4, 441-460	12.7	7
291	Machine learning for materials discovery: Two-dimensional topological insulators. *Applied Physics Reviews*, **2021**, 8, 031409	17.3	7
290	Emergent quasiparticles in Euclidean tilings. *Nanoscale*, **2021**, 13, 5270-5274	7.7	2
289	Converging Multidimensional Sensor and Machine Learning Toward High-Throughput and Biorecognition Element-Free Multidetermination of Extracellular Vesicle Biomarkers. *ACS Sensors*, **2020**, 5, 1864-1871	9.2	10

288	Pair Distribution Function from Electron Diffraction in Cryogenic Electron Microscopy: Revealing Glassy Water Structure. *Journal of Physical Chemistry Letters*, **2020**, 11, 1564-1569	6.4	9
287	Jacutingaite-family: A class of topological materials. *Physical Review B*, **2020**, 102,	3.3	3
286	Exploring Two-Dimensional Materials Thermodynamic Stability via Machine Learning. *ACS Applied Materials & Interfaces*, **2020**, 12, 20149-20157	9.5	43
285	Simulations and Materials Chemistry in the Age of Big Data. *Journal of Chemical Information and Modeling*, **2020**, 60, 452-459	6.1	18
284	Ambipolar Resistive Switching in an Ultrathin Surface-Supported Metal-Organic Framework Vertical Heterojunction. *Nano Letters*, **2020**, 20, 1080-1088	11.5	29
283	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	8.5	7
282	The Rashba Scale: Emergence of Band Anti-crossing as a Design Principle for Materials with Large Rashba Coefficient. *Matter*, **2020**, 3, 145-165	12.7	9
281	Dual topological insulator device with disorder robustness. *Physical Review B*, **2020**, 102,	3.3	6
280	Inverse design of compounds that have simultaneously ferroelectric and Rashba cofunctionality. *Physical Review B*, **2020**, 102,	3.3	6
279	Simulations of X-ray absorption spectroscopy and energetic conformation of N-heterocyclic carbenes on Au(111). *Physical Chemistry Chemical Physics*, **2020**, 22, 21504-21511	3.6	0
278	The 2021 quantum materials roadmap. *JPhys Materials*, **2020**, 3, 042006	4.2	48
277	Zeeman-type spin splitting in nonmagnetic three-dimensional compounds. *Npj Quantum Materials*, **2019**, 4,	5	13
276	Metal Chalcogenides Janus Monolayers for Efficient Hydrogen Generation by Photocatalytic Water Splitting. *ACS Applied Nano Materials*, **2019**, 2, 890-897	5.6	40
275	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	7.4	15
274	Theoretical and Experimental Investigation of 2D Hematite. *Journal of Physical Chemistry C*, **2019**, 123, 16359-16365	3.8	9
273	Electronic transport properties of MoS nanoribbons embedded in butadiene solvent. *Physical Chemistry Chemical Physics*, **2019**, 21, 11359-11366	3.6	5
272	Decreasing Nanocrystal Structural Disorder by Ligand Exchange: An Experimental and Theoretical Analysis. *Journal of Physical Chemistry Letters*, **2019**, 10, 1471-1476	6.4	9
271	From DFT to machine learning: recent approaches to materials science– review. *JPhys Materials*, **2019**, 2, 032001	4.2	206

270	Toward Realistic Amorphous Topological Insulators. *Nano Letters*, **2019**, 19, 8941-8946	11.5	19
269	The role played by the molecular geometry on the electronic transport through nanometric organic films. *Physical Chemistry Chemical Physics*, **2019**, 21, 24584-24591	3.6	2
268	Structural evolution and the role of native defects in subnanometer MoS nanowires. *Physical Review B*, **2019**, 100,	3.3	4
267	Oxidation of Ni13 clusters. *International Journal of Quantum Chemistry*, **2019**, 119, e25874	2.1	4
266	Semiclassical transport properties of IrGa: a promising thermoelectric material. *Journal of Physics Condensed Matter*, **2018**, 30, 085701	1.8	4
265	Nanoporous ZnO: Structural and electronic study under biaxial strain. *Computational Materials Science*, **2018**, 149, 91-97	3.2	
264	Tight-binding model for the band dispersion in rhombohedral topological insulators over the whole Brillouin zone. *Physical Review B*, **2018**, 98,	3.3	6
263	Layer-dependent band alignment of few layers of blue phosphorus and their van der Waals heterostructures with graphene. *Physical Review B*, **2018**, 97,	3.3	34
262	Silicene-Based FET for Logical Technology. *IEEE Electron Device Letters*, **2018**, 39, 1258-1261	4.4	7
261	Controlling Topological States in Topological/Normal Insulator Heterostructures. *ACS Omega*, **2018**, 3, 15900-15906	3.9	5
260	Band gap tuning of layered III-Te materials. *Journal of Applied Physics*, **2018**, 124, 045104	2.5	3
259	Oxidation of free-standing and supported borophene. *2D Materials*, **2017**, 4, 025025	5.9	26
258	Stacking-dependent transport properties in few-layers graphene. *Solid State Communications*, **2017**, 250, 70-74	1.6	8
257	Adsorption of 3d, 4d, and 5d transition metal atoms on □Borophene. *Journal of Physics Condensed Matter*, **2017**, 29, 305302	1.8	9
256	Tuning the p-type Schottky barrier in 2D metal/semiconductor interface:boron-sheet on MoSe, and WSe. *Journal of Physics Condensed Matter*, **2017**, 29, 405002	1.8	3
255	Nanodots of transition metal dichalcogenides embedded in MoS and MoSe: first-principles calculations. *Physical Chemistry Chemical Physics*, **2017**, 19, 26240-26247	3.6	
254	Dynamic covalent bond from first principles: Diarylbibenzofuranone structural, electronic, and oxidation studies. *Journal of Computational Chemistry*, **2017**, 38, 2675-2679	3.5	3
253	Novel III-Te□raphene van der Waals heterojunctions for optoelectronic devices. *RSC Advances*, **2017**, 7, 32383-32390	3.7	6

252	Two-dimensional van der Waals p-n junction of InSe/phosphorene. *Physical Review B*, **2017**, 95,	3.3	47
251	Directional dependence of the electronic and transport properties of 2D borophene and borophane. *Physical Chemistry Chemical Physics*, **2016**, 18, 25491-25496	3.6	77
250	Fully and partially iodinated germanane as a platform for the observation of the quantum spin Hall effect. *Physical Review B*, **2016**, 93,	3.3	13
249	Unconventional spin texture in a noncentrosymmetric quantum spin Hall insulator. *Physical Review B*, **2016**, 94,	3.3	11
248	Substrate-supported large-band-gap quantum spin Hall insulator based on III-V bismuth layers. *Physical Review B*, **2016**, 94,	3.3	1
247	A new class of large band gap quantum spin hall insulators: 2D fluorinated group-IV binary compounds. *Scientific Reports*, **2016**, 6, 26123	4.9	13
246	On the nature of the solvated electron in ice Ih. *Physical Chemistry Chemical Physics*, **2016**, 18, 4652-8	3.6	6
245	Topological states of nanoscale Bi2Se3 interfaced with AlN. *Applied Physics Letters*, **2016**, 109, 131601	3.4	4
244	Vertical twinning of the Dirac cone at the interface between topological insulators and semiconductors. *Nature Communications*, **2015**, 6, 7630	17.4	22
243	Tuning the thermoelectric properties of a single-molecule junction by mechanical stretching. *Physical Chemistry Chemical Physics*, **2015**, 17, 5386-92	3.6	11
242	Topological phase transitions of (BixSb1-x)2Se3 alloys by density functional theory. *Journal of Physics Condensed Matter*, **2015**, 27, 255501	1.8	9
241	Valley Hall effect in silicene and hydrogenated silicene ruled by grain boundaries: An ab initio investigation. *Physical Review B*, **2015**, 91,	3.3	8
240	Van der Waals heterostructure of phosphorene and graphene: tuning the Schottky barrier and doping by electrostatic gating. *Physical Review Letters*, **2015**, 114, 066803	7.4	372
239	Switching a normal insulator into a topological insulator via electric field with application to phosphorene. *Nano Letters*, **2015**, 15, 1222-8	11.5	343
238	Size- effect induced high thermoelectric figure of merit in PbSe and PbTe nanowires. *Physical Chemistry Chemical Physics*, **2014**, 16, 8114-8	3.6	11
237	Directional Control of the Electronic and Transport Properties of Graphynes. *Journal of Physical Chemistry C*, **2014**, 118, 18793-18798	3.8	16
236	Quantum spin Hall effect on germanene nanorod embedded in completely hydrogenated germanene. *Physical Review B*, **2014**, 89,	3.3	46
235	First-principles study of HgTe/CdTe heterostructures under perturbations preserving time-reversal symmetry. *Physical Review B*, **2014**, 90,	3.3	9

234	Spin caloritronics in graphene with Mn. *Applied Physics Letters*, **2014**, 104, 072412	3.4	15
233	Topological phases in triangular lattices of Ru adsorbed on graphene: Ab initio calculations. *Physical Review B*, **2014**, 89,	3.3	23
232	Graphene on amorphous HfO2 surface: An ab initio investigation. *Physical Review B*, **2013**, 87,	3.3	11
231	Graphene nanoribbon intercalated with hexagonal boron nitride: Electronic transport properties from ab initio calculations. *Solid State Communications*, **2013**, 173, 24-29	1.6	10
230	Topological insulator Bi2Se3(111) surface doped with transition metals: An ab initio investigation. *Physical Review B*, **2013**, 88,	3.3	46
229	Electronic transport in patterned graphene nanoroads. *Nanotechnology*, **2013**, 24, 495201	3.4	8
228	Quantum spin Hall effect in a disordered hexagonal SixGe1−x alloy. *Physical Review B*, **2013**, 88,	3.3	21
227	Topological states ruled by stacking faults in Bi2Se3 and Bi2Te3. *Journal of Applied Physics*, **2013**, 113, 023705	2.5	19
226	Confinement effects and why carbon nanotube bundles can work as gas sensors. *Nanoscale*, **2013**, 5, 2798-803	7.7	22
225	First-principles study of group III impurity doped PbSe: Bulk and nanowire. *Physical Review B*, **2013**, 87,	3.3	6
224	Carrier-mediated magnetism in transition metal doped Bi2Se3 topological insulator. *Journal of Physics Condensed Matter*, **2013**, 25, 445003	1.8	5
223	Interfaces between buckling phases in silicene: Ab initio density functional theory calculations. *Physical Review B*, **2013**, 88,	3.3	10
222	Considerações sobre o Programa Brasileiro de Nanotecnologia. *Ciência E Cultura*, **2013**, 65, 23-27	0.3	1
221	Tuning Low-Spin to High-Spin Mn Pairs in 2-D ZnO by Injecting Holes. *IEEE Nanotechnology Magazine*, **2012**, 11, 71-76	2.6	0
220	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	1.8	15
219	Light emission and current rectification in a molecular device: Experiment and theory. *Journal of Applied Physics*, **2012**, 112, 113108	2.5	
218	Ab-initio calculations for a realistic sensor: A study of CO sensors based on nitrogen-rich carbon nanotubes. *AIP Advances*, **2012**, 2, 032115	1.5	4
217	Piezomagnetic behavior of Co-doped ZnO nanoribbons. *Physical Review B*, **2011**, 84,	3.3	5

216	Doping of graphene adsorbed on the a-SiO2 surface. *Applied Physics Letters*, **2011**, 99, 163108	3.4	43
215	Mn dimers on graphene nanoribbons: An ab initio study. *Journal of Applied Physics*, **2011**, 109, 053715	2.5	14
214	Quantum confinement and spin-orbit interactions in PbSe and PbTe nanowires: First-principles calculation. *Physical Review B*, **2011**, 84,	3.3	9
213	Bilayer graphene dual-gate nanodevice: An ab initio simulation. *Physical Review B*, **2011**, 84,	3.3	29
212	Spin filtering and disorder-induced magnetoresistance in carbon nanotubes: Ab initio calculations. *Physical Review B*, **2011**, 84,	3.3	13
211	Spin texture and magnetic anisotropy of Co impurities in Bi2Se3 topological insulators. *Physical Review B*, **2011**, 84,	3.3	45
210	Electronic transport properties of ascorbic acid and nicotinamide adsorbed on single-walled carbon nanotubes. *Chemical Physics Letters*, **2011**, 506, 233-238	2.5	10
209	IxV curves of boron and nitrogen doping zigzag graphene nanoribbons. *International Journal of Quantum Chemistry*, **2011**, 111, 1379-1386	2.1	16
208	Adatoms in graphene as a source of current polarization: Role of the local magnetic moment. *Physical Review B*, **2011**, 84,	3.3	25
207	Ab initio calculations of structural evolution and conductance of benzene-1,4-dithiol on gold leads. *ACS Nano*, **2011**, 5, 795-804	16.7	83
206	Energetics and stability of vacancies in carbon nanotubes. *Solid State Communications*, **2011**, 151, 482-486	1.6	37
205	Mn-doped cubic BN as an atomiclike memory device: A density functional study. *Physical Review B*, **2010**, 81,	3.3	2
204	Splitting of the zero-energy edge states in bilayer graphene. *Physical Review B*, **2010**, 81,	3.3	12
203	Disorder-based graphene spintronics. *Nanotechnology*, **2010**, 21, 345202	3.4	27
202	Origin of FM ordering in pristine micro- and nanostructured ZnO. *Nano Letters*, **2010**, 10, 1383-6	11.5	92
201	Ferromagnetic coupling in a Co-doped graphenelike ZnO sheet. *Physical Review B*, **2010**, 81,	3.3	54
200	Mimicking nanoribbon behavior using a graphene layer on SiC. *Physical Review B*, **2010**, 82,	3.3	8
199	Surface and Quantum Confinement Effects in ZnO Nanocrystals. *Journal of Physical Chemistry C*, **2010**, 114, 18293-18297	3.8	45

198	Formation of atomic carbon chains from graphene nanoribbons. *Physical Review B*, **2010**, 81,	3.3	50
197	Realistic calculations of carbon-based disordered systems. *Journal Physics D: Applied Physics*, **2010**, 43, 374002	3	18
196	Organic molecule assembled between carbon nanotubes: A highly efficient switch device. *Physical Review B*, **2009**, 79,	3.3	34
195	Point defects in covalent semiconductors: A molecular cluster model. *International Journal of Quantum Chemistry*, **2009**, 16, 349-361	2.1	1
194	The variational cellular method for quantum mechanical applications: Calculations of the ground and excited states of F2 and Ne2 molecules. *International Journal of Quantum Chemistry*, **2009**, 20, 401-408	2.1	
193	MS-X□Treatment for native defects in GaSb. *International Journal of Quantum Chemistry*, **2009**, 20, 457-457	2.1	
192	Native defects and transition metal impurities at interstitial sites in gaas. *International Journal of Quantum Chemistry*, **2009**, 36, 677-685	2.1	
191	Metal-semiconductor transition in cerium hydrides. *International Journal of Quantum Chemistry*, **2009**, 36, 709-716	2.1	
190	Surface magnetization in non-doped ZnO nanostructures. *Applied Physics Letters*, **2009**, 94, 162503	3.4	67
189	Electronic, structural, and transport properties of Ni-doped graphene nanoribbons. *Physical Review B*, **2009**, 79,	3.3	130
188	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, 5376-80	3.4	10
187	Edge effects in bilayer graphene nanoribbons: Ab initio total-energy density functional theory calculations. *Physical Review B*, **2009**, 79,	3.3	54
186	Barrier-free substitutional doping of graphene sheets with boron atoms: Ab initio calculations. *Physical Review B*, **2009**, 79,	3.3	57
185	Theoretical investigation of Hf and Zr defects in c-Ge. *Journal of Physics Condensed Matter*, **2009**, 21, 012206	1.8	
184	Quantum confinement effects on Mn-doped InAs nanocrystals: A first-principles study. *Physical Review B*, **2008**, 78,	3.3	17
183	Hydrogen adsorption on boron doped graphene: an ab initio study. *Nanotechnology*, **2008**, 19, 155708	3.4	80
182	First-principles study of the adsorption of atomic and molecular hydrogen on BC2N nanotubes. *Physical Review B*, **2008**, 77,	3.3	29
181	sigma- and pi-defects at graphene nanoribbon edges: building spin filters. *Nano Letters*, **2008**, 8, 2293-8	11.5	94

180	Confinement and surface effects in B and P doping of silicon nanowires. *Nano Letters*, **2008**, 8, 1866-71	11.5	53
179	Electronic and Magnetic Properties of Ti and Fe on Graphene. *Journal of Physical Chemistry C*, **2008**, 112, 9163-9167	3.8	83
178	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	3.8	4
177	Symmetry controlled spin polarized conductance in au nanowires. *Journal of the American Chemical Society*, **2008**, 130, 9897-903	16.4	20
176	Designing real nanotube-based gas sensors. *Physical Review Letters*, **2008**, 100, 176803	7.4	95
175	Amorphous HfO2 and Hf1−xSixO via a melt-and-quench scheme using ab initio molecular dynamics. *Physical Review B*, **2008**, 77,	3.3	39
174	Transport properties of single vacancies in nanotubes. *Physical Review B*, **2008**, 77,	3.3	32
173	Temperature and quantum effects in the stability of pure and doped gold nanowires. *Physical Review Letters*, **2008**, 100, 056104	7.4	29
172	Divacancies in graphene and carbon nanotubes. *Nano Letters*, **2007**, 7, 2459-62	11.5	151
171	Si nanowires as sensors: choosing the right surface. *Nano Letters*, **2007**, 7, 1172-7	11.5	37
170	Electronic and transport properties of boron-doped graphene nanoribbons. *Physical Review Letters*, **2007**, 98, 196803	7.4	502
169	Adsorption of CO and NO molecules on carbon doped boron nitride nanotubes. *Solid State Communications*, **2007**, 142, 49-53	1.6	96
168	First principles study of titanium-coated carbon nanotubes as sensors for carbon monoxide molecules. *Surface Science*, **2007**, 601, 4102-4104	1.8	22
167	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	2.5	34
166	Ab initio study of pristine and Si-doped capped carbon nanotubes interacting with nimesulide molecules. *Chemical Physics Letters*, **2007**, 439, 348-353	2.5	34
165	Simple implementation of complex functionals: scaled self-consistency. *Journal of Chemical Physics*, **2007**, 126, 144107	3.9	7
164	Theoretical investigations of Ge nanowires grown along the [110] and [111] directions. *Nanotechnology*, **2007**, 18, 295706	3.4	28
163	Theoretical investigation of a Mn-doped Si□e heterostructure. *Physical Review B*, **2007**, 75,	3.3	9

162	Hf defects in cSi and their importance for the HfO2Si interface: Density-functional calculations. *Physical Review B*, **2007**, 75,	3.3	4
161	EL2-like defects in InP nanowires: An ab initio total energy investigation. *Physical Review B*, **2007**, 75,	3.3	6
160	Structural, electronic, and magnetic properties of Mn-doped Ge nanowires by ab initio calculations. *Physical Review B*, **2007**, 75,	3.3	16
159	Short linear atomic chains in copper nanowires. *Nanotechnology*, **2007**, 18, 145701	3.4	30
158	Gold nanowires and the effect of impurities. *Nanoscale Research Letters*, **2006**, 1, 91-98	5	16
157	Titanium monomers and wires adsorbed on carbon nanotubes: a first principles study. *Nanotechnology*, **2006**, 17, 1154-9	3.4	22
156	Orientational defects in ice Ih: an interpretation of electrical conductivity measurements. *Physical Review Letters*, **2006**, 96, 075501	7.4	34
155	Structure and energetics of molecular point defects in ice Ih. *Physical Review Letters*, **2006**, 97, 155501	7.4	21
154	Electronic and magnetic properties of Mn-doped InP nanowires from first principles. *Physical Review B*, **2006**, 73,	3.3	27
153	Oxygen clamps in gold nanowires. *Physical Review Letters*, **2006**, 96, 016104	7.4	60
152	Hydrogen adsorption on carbon-doped boron nitride nanotube. *Journal of Physical Chemistry B*, **2006**, 110, 21184-8	3.4	89
151	C59Si on the monohydride Si(100):H-(2 x 1) surface. *Journal of Physical Chemistry B*, **2006**, 110, 10849-54	3.4	8
150	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, 8996-7	16.4	63
149	First principles calculations of as impurities in the presence of a 90° partial dislocation in Si. *Brazilian Journal of Physics*, **2006**, 36, 261-263	1.2	6
148	Density functional theory method for non-equilibrium charge transport calculations: TRANSAMPA. *Brazilian Journal of Physics*, **2006**, 36, 799-807	1.2	51
147	Phenomenological band structure model of magnetic coupling in semiconductors. *Solid State Communications*, **2006**, 138, 353-358	1.6	117
146	Silicon adsorption in defective carbon nanotubes: a first principles study. *Nanotechnology*, **2006**, 17, 4088-91	3.4	4
145	Stability and electronic confinement of free-standing InP nanowires: Ab initio calculations. *Physical Review B*, **2005**, 72,	3.3	35

144	Bundling up carbon nanotubes through Wigner defects. *Nano Letters*, **2005**, 5, 1045-9	11.5	32
143	Vacancy formation process in carbon nanotubes: first-principles approach. *Nano Letters*, **2005**, 5, 197-200	11.5	72
142	Carbon nanotube adsorbed on hydrogenated Si(001) surfaces. *Applied Surface Science*, **2005**, 244, 124-128	1.7	5
141	Computer simulations in the study of gold nanowires: the effect of impurities. *Applied Physics A: Materials Science and Processing*, **2005**, 81, 1551-1558	2.6	15
140	Electronic and structural properties of C59Si on the monohydride Si(100) surface. *International Journal of Quantum Chemistry*, **2005**, 103, 557-561	2.1	2
139	Comment on "contaminants in suspended gold chains: an Ab initio molecular dynamics study.". *Physical Review Letters*, **2005**, 95, 169601; author reply 169602	7.4	11
138	Disorder and the effective MnMn exchange interaction in Ga1−xMnxAs diluted magnetic semiconductors. *Physical Review B*, **2005**, 72,	3.3	13
137	Oxygen-induced atomic desorptions in oxynitrides: Density functional calculations. *Physical Review B*, **2005**, 72,	3.3	5
136	Substrate-dependent electronic properties of an armchair carbon nanotube adsorbed on HSi(001). *Applied Physics Letters*, **2005**, 86, 213111	3.4	33
135	Formation energy of native defects in BN nanotubes: anab initiostudy. *Nanotechnology*, **2005**, 16, 827-831	1.4	69
134	Anab initiostudy of manganese atoms and wires interacting with carbon nanotubes. *Journal of Physics Condensed Matter*, **2004**, 16, 3647-3661	1.8	15
133	Stabilization of substitutional Mn in silicon-based semiconductors. *Physical Review B*, **2004**, 70,	3.3	38
132	Initial stages of Ge and Si growth near SB monoatomic steps on Si(100). *Physical Review B*, **2004**, 70,	3.3	3
131	Theoretical study of the formation, evolution, and breaking of gold nanowires. *Physical Review B*, **2004**, 69,	3.3	101
130	Carbon in SixGe1−x: An ab initio investigation. *Physical Review B*, **2004**, 69,	3.3	8
129	Diffusion-reaction mechanisms of nitriding species in SiO2. *Physical Review B*, **2004**, 70,	3.3	20
128	Adsorption of Mn atoms on the Si(1 0 0) surface. *Surface Science*, **2004**, 566-568, 688-692	1.8	9
127	Stability and electronic properties of carbon nanotubes adsorbed on Si(0 0 1). *Surface Science*, **2004**, 566-568, 728-732	1.8	15

126	Effect of impurities on the breaking of Au nanowires. *Surface Science*, **2004**, 566-568, 367-371	1.8	6
125	Substitutional Si Doping in Deformed Carbon Nanotubes. *Nano Letters*, **2004**, 4, 975-977	11.5	38
124	First principles study of the ferromagnetism in Ga1−xMnxAs semiconductors. *Journal of Physics Condensed Matter*, **2004**, 16, 8243-8250	1.8	15
123	Comparative study of defect energetics in HfO2 and SiO2. *Applied Physics Letters*, **2004**, 84, 1492-1494	3.4	102
122	Breaking of gold nanowires. *Computational Materials Science*, **2004**, 30, 73-76	3.2	18
121	On the reversibility of hydrogen effects on the properties of amorphous silicon carbide. *Journal of Non-Crystalline Solids*, **2004**, 338-340, 299-302	3.9	4
120	Vacancy-like defects in a-Si: a first principles study. *Journal of Non-Crystalline Solids*, **2004**, 338-340, 400-402	3.9	9
119	First-principles calculations of carbon nanotubes adsorbed on Si(001). *Physical Review Letters*, **2003**, 91, 166802	7.4	50
118	Electronic structure and origin of ferromagnetism in Ga1−xMnxAs semiconductors. *Physica B: Condensed Matter*, **2003**, 340-342, 874-877	2.8	9
117	Energetics and structural properties of adsorbed atoms and molecules on silicon-doped carbon nanotubes. *Materials Characterization*, **2003**, 50, 183-187	3.9	23
116	Fe and Mn atoms interacting with carbon nanotubes. *Physica B: Condensed Matter*, **2003**, 340-342, 982-985	2.8	19
115	Electronic and magnetic properties of iron chains on carbon nanotubes. *Microelectronics Journal*, **2003**, 34, 481-484	1.8	32
114	Theoretical study of native defects in BN nanotubes. *Physical Review B*, **2003**, 67,	3.3	143
113	Oxidation at the Si/SiO2 interface: influence of the spin degree of freedom. *Physical Review Letters*, **2003**, 90, 016103	7.4	29
112	Ab initio study of an iron atom interacting with single-wall carbon nanotubes. *Physical Review B*, **2003**, 67,	3.3	94
111	Ab initio study of an organic molecule interacting with a silicon-doped carbon nanotube. *Diamond and Related Materials*, **2003**, 12, 861-863	3.5	17
110	Effect of impurities in the large Au-Au distances in gold nanowires. *Physical Review Letters*, **2003**, 90, 036101	7.4	69
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