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	Electronic and Transport Properties of Boron-Doped Graphene Nanoribbons. Physical Review Letters, 2007, 98, 196803.	2.9	540
2	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
3	Switching a Normal Insulator into a Topological Insulator via Electric Field with Application to Phosphorene. Nano Letters, 2015, 15, 1222-1228.	4.5	406
4	From DFT to machine learning: recent approaches to materials scienceâ€“a review. JPhys Materials, 2019, 2, 032001.	1.8	385
5	A universal trend in the binding energies of deep impurities in semiconductors. Applied Physics Letters, 1984, 45, 671-673.	1.5	256
6	Many-electron multiplet effects in the spectra of3dimpurities in heteropolar semiconductors. Physical Review B, 1984, 30, 3430-3455.	1.1	250
7	Ab initiocalculations for a hypothetical material: Silicon nanotubes. Physical Review B, 2000, 61, 9994-9996.	1.1	240
8	How Do Gold Nanowires Break?. Physical Review Letters, 2001, 87, 256102.	2.9	208
9	Divacancies in Graphene and Carbon Nanotubes. Nano Letters, 2007, 7, 2459-2462.	4.5	175
10	Theoretical study of native defects in BN nanotubes. Physical Review B, 2003, 67, .	1.1	151
11	Electronic, structural, and transport properties of Ni-doped graphene nanoribbons. Physical Review B, 2009, 79, .	1.1	143
12	Structural properties of amorphous silicon nitride. Physical Review B, 1998, 58, 8323-8328.	1.1	140
13	Phenomenological band structure model of magnetic coupling in semiconductors. Solid State Communications, 2006, 138, 353-358.	0.9	134
14	Comparative study of defect energetics in HfO2 and SiO2. Applied Physics Letters, 2004, 84, 1492-1494.	1.5	113
15	Adsorption of CO and NO molecules on carbon doped boron nitride nanotubes. Solid State Communications, 2007, 142, 49-53.	0.9	112
16	The 2021 quantum materials roadmap. JPhys Materials, 2020, 3, 042006.	1.8	111
17	Theoretical study of the formation, evolution, and breaking of gold nanowires. Physical Review B, 2004, 69, .	1.1	110
18	Electronic and structural properties of silicon-doped carbon nanotubes. Physical Review B, 2001, 64, .	1.1	109

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19	Hydrogen Adsorption on Carbon-Doped Boron Nitride Nanotube. Journal of Physical Chemistry B, 2006, 110, 21184-21188.	1.2	105
20	Designing Real Nanotube-Based Gas Sensors. Physical Review Letters, 2008, 100, 176803.	2.9	102
21	Ab initiostudy of an iron atom interacting with single-wall carbon nanotubes. Physical Review B, 2003, 67, .	1.1	101
22	Ïƒ- and Ï€-Defects at Graphene Nanoribbon Edges: Building Spin Filters. Nano Letters, 2008, 8, 2293-2298.	4.5	101
23	Origin of FM Ordering in Pristine Micro- and Nanostructured ZnO. Nano Letters, 2010, 10, 1383-1386.	4.5	98
24	Stability investigation and thermal behavior of a hypothetical silicon nanotube. Computational and Theoretical Chemistry, 2001, 539, 101-106.	1.5	93
25	Metal Chalcogenides Janus Monolayers for Efficient Hydrogen Generation by Photocatalytic Water Splitting. ACS Applied Nano Materials, 2019, 2, 890-897.	2.4	93
26	Directional dependence of the electronic and transport properties of 2D borophene and borophane. Physical Chemistry Chemical Physics, 2016, 18, 25491-25496.	1.3	92
27	Electronic and Magnetic Properties of Ti and Fe on Graphene. Journal of Physical Chemistry C, 2008, 112, 9163-9167.	1.5	91
28	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
29	Hydrogen role on the properties of amorphous silicon nitride. Journal of Applied Physics, 1999, 86, 1843-1847.	1.1	88
30	Hydrogen adsorption on boron doped graphene: anab initiostudy. Nanotechnology, 2008, 19, 155708.	1.3	86
31	Microscopic picture of the single vacancy in germanium. Physical Review B, 2000, 61, R2401-R2404.	1.1	82
32	Exploring Two-Dimensional Materials Thermodynamic Stability via Machine Learning. ACS Applied Materials & Interfaces, 2020, 12, 20149-20157.	4.0	80
33	Electronic structure of copper, silver, and gold impurities in silicon. Physical Review B, 1985, 32, 934-954.	1.1	76
34	Effect of Impurities in the Large Au-Au Distances in Gold Nanowires. Physical Review Letters, 2003, 90, 036101.	2.9	76
35	Vacancy Formation Process in Carbon Nanotubes:Â First-Principles Approach. Nano Letters, 2005, 5, 197-200.	4.5	76
36	Formation energy of native defects in BN nanotubes: anab initiostudy. Nanotechnology, 2005, 16, 827-831.	1.3	74

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37	Surface magnetization in non-doped ZnO nanostructures. Applied Physics Letters, 2009, 94, .	1.5	74
38	Two-dimensional van der Waals p-n junction of InSe/phosphorene. Physical Review B, 2017, 95, .	1.1	68
39	Electronic structure of Cu, Ni, Co, and Fe substitutional impurities in gallium arsenide. Physical Review B, 1980, 21, 4710-4720.	1.1	67
40	Functionalization of carbon nanotubes through the chemical binding of atoms and molecules. Physical Review B, 2003, 67, .	1.1	67
41	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
42	Oxygen Clamps in Gold Nanowires. Physical Review Letters, 2006, 96, 016104.	2.9	64
43	Barrier-free substitutional doping of graphene sheets with boron atoms:Ab initiocalculations. Physical Review B, 2009, 79, .	1.1	63
44	Ferromagnetic coupling in a Co-doped graphenelike ZnO sheet. Physical Review B, 2010, 81, .	1.1	62
45	Self-interstitial defect in germanium. Physical Review B, 2000, 62, 9903-9906.	1.1	59
46	Edge effects in bilayer graphene nanoribbons:Ab initiototal-energy density functional theory calculations. Physical Review B, 2009, 79, .	1.1	58
47	Ab initiodetermination of the atomistic structure ofSixGe1â^'xalloy. Physical Review B, 2001, 64, .	1.1	57
48	Quantum spin Hall effect on germanene nanorod embedded in completely hydrogenated germanene. Physical Review B, 2014, 89, .	1.1	57
49	First-Principles Calculations of Carbon Nanotubes Adsorbed on Si(001). Physical Review Letters, 2003, 91, 166802.	2.9	54
50	Formation of atomic carbon chains from graphene nanoribbons. Physical Review B, 2010, 81, .	1.1	54
51	Confinement and Surface Effects in B and P Doping of Silicon Nanowires. Nano Letters, 2008, 8, 1866-1871.	4.5	53
52	Surface and Quantum Confinement Effects in ZnO Nanocrystals. Journal of Physical Chemistry C, 2010, 114, 18293-18297.	1.5	53
53	Ambipolar Resistive Switching in an Ultrathin Surface-Supported Metalâ€“Organic Framework Vertical Heterojunction. Nano Letters, 2020, 20, 1080-1088.	4.5	53
54	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

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55	Density functional theory method for non-equilibrium charge transport calculations: TRANSAMPA. Brazilian Journal of Physics, 2006, 36, 799-807.	0.7	51
56	Anion-antisite-like defects in III-V compounds. Physical Review Letters, 1990, 65, 2046-2049.	2.9	50
57	Substitutional Si Doping in Deformed Carbon Nanotubes. Nano Letters, 2004, 4, 975-977.	4.5	48
58	Multiple scattering-XÎ± cluster model of GaAs: electronic states of isolated vacancies and substitutional impurities. Journal of Physics C: Solid State Physics, 1979, 12, 3469-3481.	1.5	47
59	Separation of one- and many-electron effects in the excitation spectra of3dimpurities in semiconductors. Physical Review B, 1984, 29, 5999-6002.	1.1	47
60	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
61	AmorphousHfO2andHf1â^'xSixOvia a melt-and-quench scheme usingab initiomolecular dynamics. Physical Review B, 2008, 77, .	1.1	46
62	Doping of graphene adsorbed on the a-SiO2 surface. Applied Physics Letters, 2011, 99, 163108.	1.5	46
63	First-principles investigation ofaâ^'SiNx:H. Physical Review B, 2002, 65, .	1.1	45
64	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
65	Toward Realistic Amorphous Topological Insulators. Nano Letters, 2019, 19, 8941-8946.	4.5	44
66	Theoretical investigation of a possibleMnxSi1â^'xferromagnetic semiconductor. Physical Review B, 2003, 68, .	1.1	42
67	Energetics and stability of vacancies in carbon nanotubes. Solid State Communications, 2011, 151, 482-486.	0.9	42
68	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
69	Si Nanowires as Sensors:Â Choosing the Right Surface. Nano Letters, 2007, 7, 1172-1177.	4.5	40
70	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
71	O2 Diffusion in SiO2: Triplet versus Singlet. Physical Review Letters, 2001, 87, 155901.	2.9	38
72	Stabilization of substitutional Mn in silicon-based semiconductors. Physical Review B, 2004, 70, .	1.1	38

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73	Electronic and structural trends in small GaAs clusters. Scripta Materialia, 1998, 10, 635-647.	0.5	36
74	Optical Transitions in Ruby across the Corundum toRh2O3(II) Phase Transformation. Physical Review Letters, 1998, 81, 3267-3270.	2.9	36
75	Organic molecule assembled between carbon nanotubes: A highly efficient switch device. Physical Review B, 2009, 79, .	1.1	36
76	Bilayer graphene dual-gate nanodevice: Anab initiosimulation. Physical Review B, 2011, 84, .	1.1	36
77	Stability and electronic confinement of free-standingInPnanowires:Ab initiocalculations. Physical Review B, 2005, 72, .	1.1	35
78	Orientational Defects in Ice Ih: An Interpretation of Electrical Conductivity Measurements. Physical Review Letters, 2006, 96, 075501.	2.9	35
79	Transport properties of single vacancies in nanotubes. Physical Review B, 2008, 77, .	1.1	35
80	A molecular cluster model of the electronic structure of IV and III-V covalent semiconductors: Application to GaAs. Journal of Physics C: Solid State Physics, 1979, 12, 513-524.	1.5	34
81	Electronic and magnetic properties of iron chains on carbon nanotubes. Microelectronics Journal, 2003, 34, 481-484.	1.1	34
82	Substrate-dependent electronic properties of an armchair carbon nanotube adsorbed on Hâˆ•Si(001). Applied Physics Letters, 2005, 86, 213111.	1.5	34
83	Machine learning for materials discovery: Two-dimensional topological insulators. Applied Physics Reviews, 2021, 8, .	5.5	34
84	Oxidation at theSi/SiO2Interface: Influence of the Spin Degree of Freedom. Physical Review Letters, 2003, 90, 016103.	2.9	33
85	Short linear atomic chains in copper nanowires. Nanotechnology, 2007, 18, 145701.	1.3	33
86	Theoretical investigation of the electrical and optical activity of vanadium in GaAs. Physical Review B, 1986, 33, 7102-7109.	1.1	32
87	Point defect interactions with extended defects in semiconductors. Physical Review B, 1999, 60, 4711-4714.	1.1	32
88	Vacancy-mediated diffusion in disordered alloys: Ge self-diffusion inSi1âˆ’xGex. Physical Review B, 2002, 65, .	1.1	32
89	Bundling up Carbon Nanotubes through Wigner Defects. Nano Letters, 2005, 5, 1045-1049.	4.5	32
90	Theoretical investigations of Ge nanowires grown along the [110] and [111] directions. Nanotechnology, 2007, 18, 295706.	1.3	31

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91	Oxidation of free-standing and supported borophene. 2D Materials, 2017, 4, 025025.	2.0	31
92	Electronic and magnetic properties of Mn-doped InP nanowires from first principles. Physical Review B, 2006, 73, .	1.1	30
93	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
94	Temperature and Quantum Effects in the Stability of Pure and Doped Gold Nanowires. Physical Review Letters, 2008, 100, 056104.	2.9	30
95	Disorder-based graphene spintronics. Nanotechnology, 2010, 21, 345202.	1.3	30
96	Pair Distribution Function Obtained from Electron Diffraction: An Advanced Real-Space Structural Characterization Tool. Matter, 2021, 4, 441-460.	5.0	29
97	Theoretical studies of native defects in cubic boron nitride. Physical Review B, 1997, 56, 3556-3559.	1.1	28
98	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
99	Role played by N and N-N impurities in type-IV semiconductors. Physical Review B, 1993, 48, 17806-17810.	1.1	27
100	Adatoms in graphene as a source of current polarization: Role of the local magnetic moment. Physical Review B, 2011, 84, .	1.1	27
101	Vertical twinning of the Dirac cone at the interface between topological insulators and semiconductors. Nature Communications, 2015, 6, 7630.	5.8	26
102	Confinement effects and why carbon nanotube bundles can work as gas sensors. Nanoscale, 2013, 5, 2798.	2.8	25
103	Topological phases in triangular lattices of Ru adsorbed on graphene:Ab initiocalculations. Physical Review B, 2014, 89, .	1.1	25
104	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
105	Energetics and structural properties of adsorbed atoms and molecules on silicon-doped carbon nanotubes. Materials Characterization, 2003, 50, 183-187.	1.9	24
106	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
107	Dislocation core properties in semiconductors. Solid State Communications, 2001, 118, 651-655.	0.9	23
108	First principles study of titanium-coated carbon nanotubes as sensors for carbon monoxide molecules. Surface Science, 2007, 601, 4102-4104.	0.8	23

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109	Zeeman-type spin splitting in nonmagnetic three-dimensional compounds. Npj Quantum Materials, 2019, 4, .	1.8	23
110	Theoretical model of the Au-Fe complex in silicon. Physical Review B, 1985, 32, 8085-8091.	1.1	22
111	Structural and electronic properties of silicon nitride materials. International Journal of Quantum Chemistry, 1998, 70, 973-980.	1.0	22
112	Titanium monomers and wires adsorbed on carbon nanotubes: a first principles study. Nanotechnology, 2006, 17, 1154-1159.	1.3	22
113	Structure and Energetics of Molecular Point Defects in Icelh. Physical Review Letters, 2006, 97, 155501.	2.9	22
114	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
115	Unconventional spin texture in a noncentrosymmetric quantum spin Hall insulator. Physical Review B, 2016, 94, .	1.1	22
116	Ab initio study of an organic molecule interacting with a silicon-doped carbon nanotube. Diamond and Related Materials, 2003, 12, 861-863.	1.8	21
117	Topological states ruled by stacking faults in Bi2Se3 and Bi2Te3. Journal of Applied Physics, 2013, 113, 023705.	1.1	21
118	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
119	Electronic and structural properties of vacancy and self-interstitial defects in germanium. Physica B: Condensed Matter, 1999, 273-274, 575-578.	1.3	20
120	Structural order and clustering in annealedÎ±â^'SiCandÎ±â^'SiC:H. Physical Review B, 2002, 65, .	1.1	20
121	Fe and Mn atoms interacting with carbon nanotubes. Physica B: Condensed Matter, 2003, 340-342, 982-985.	1.3	20
122	Diffusion-reaction mechanisms of nitriding species inSiO2. Physical Review B, 2004, 70, .	1.1	20
123	Breaking of gold nanowires. Computational Materials Science, 2004, 30, 73-76.	1.4	20
124	Symmetry Controlled Spin Polarized Conductance in Au Nanowires. Journal of the American Chemical Society, 2008, 130, 9897-9903.	6.6	20
125	Inverse design of compounds that have simultaneously ferroelectric and Rashba cofunctionality. Physical Review B, 2020, 102, .	1.1	20
126	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

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127	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
128	Effects of extended defects on the properties of intrinsic and extrinsic point defects in silicon. Physica B: Condensed Matter, 1999, 273-274, 473-475.	1.3	19
129	Theoretical investigation of the pressure induced cubic-diamond-î²-tin phase transition in the Si0.5Ge0.5. Solid State Communications, 2001, 120, 369-373.	0.9	19
130	Realistic calculations of carbon-based disordered systems. Journal Physics D: Applied Physics, 2010, 43, 374002.	1.3	19
131	Decreasing Nanocrystal Structural Disorder by Ligand Exchange: An Experimental and Theoretical Analysis. Journal of Physical Chemistry Letters, 2019, 10, 1471-1476.	2.1	19
132	Quantum confinement effects on Mn-doped InAs nanocrystals: A first-principles study. Physical Review B, 2008, 78, .	1.1	18
133	Spin caloritronics in graphene with Mn. Applied Physics Letters, 2014, 104, .	1.5	18
134	Directional Control of the Electronic and Transport Properties of Graphynes. Journal of Physical Chemistry C, 2014, 118, 18793-18798.	1.5	18
135	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
136	Formation and structural properties of the amorphous-crystal interface in a nanocrystalline system. Physical Review B, 2001, 64, .	1.1	17
137	Stability and electronic properties of carbon nanotubes adsorbed on Si(001). Surface Science, 2004, 566-568, 728-732.	0.8	17
138	Gold nanowires and the effect of impurities. Nanoscale Research Letters, 2006, 1, 91-98.	3.1	17
139	IxV curves of boron and nitrogen doping zigzag graphene nanoribbons. International Journal of Quantum Chemistry, 2011, 111, 1379-1386.	1.0	17
140	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
141	Theoretical and Experimental Investigation of 2D Hematite. Journal of Physical Chemistry C, 2019, 123, 16359-16365.	1.5	17
142	Dislocation core reconstruction in zinc-blende semiconductors. Journal of Physics Condensed Matter, 2000, 12, 10039-10044.	0.7	16
143	Anab initiostudy of manganese atoms and wires interacting with carbon nanotubes. Journal of Physics Condensed Matter, 2004, 16, 3647-3661.	0.7	16
144	Structural, electronic, and magnetic properties of Mn-doped Ge nanowires byab initiocalculations. Physical Review B, 2007, 75, .	1.1	16

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145	Adsorption of 3d, 4d, and 5dtransition metal atoms onÎ²₁₂â€"Borophene. Journal of Physics Condensed Matter, 2017, 29, 305302.	0.7	16
146	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
147	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
148	Structural and electronic properties of realistic two-dimensional amorphous topological insulators. 2D Materials, 2021, 8, 025032.	2.0	16
149	First principles study of the ferromagnetism in Ga1ÂxMnxAs semiconductors. Journal of Physics Condensed Matter, 2004, 16, 8243-8250.	0.7	15
150	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
151	Mn dimers on graphene nanoribbons: An ab initio study. Journal of Applied Physics, 2011, 109, 053715.	1.1	15
152	Size- effect induced high thermoelectric figure of merit in PbSe and PbTe nanowires. Physical Chemistry Chemical Physics, 2014, 16, 8114-8118.	1.3	15
153	Discovery of higher-order topological insulators using the spin Hall conductivity as a topology signature. Npj Computational Materials, 2021, 7, .	3.5	15
154	Many-electron treatment of the off-center substitutional O in Si. Physical Review B, 1986, 33, 4432-4435.	1.1	14
155	Ab initio calculations of vacancies in SixGe1â^'x. Applied Physics Letters, 2002, 81, 3383-3385.	1.5	14
156	Splitting of the zero-energy edge states in bilayer graphene. Physical Review B, 2010, 81, .	1.1	14
157	Spin filtering and disorder-induced magnetoresistance in carbon nanotubes:Ab initiocalculations. Physical Review B, 2011, 84, .	1.1	14
158	First-principles study of HgTe/CdTe heterostructures under perturbations preserving time-reversal symmetry. Physical Review B, 2014, 90, .	1.1	14
159	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
160	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, .	1.1	14
161	Multiple-scatteringXÎ±molecular-cluster model of complex defects in semiconductors: Application to Si:P2and Si:P2+systems. Physical Review B, 1982, 25, 2603-2610.	1.1	13
162	Electronic structure of neutral and negatively charged gallium vacancies in GaP. Journal of Physics C: Solid State Physics, 1982, 15, L1-L3.	1.5	13

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163	Interaction of As impurities with 30Â° partial dislocations in Si: An ab initio investigation. Journal of Applied Physics, 2002, 91, 5892-5895.	1.1	13
164	Disorder and the effectiveMnâ^'Mnexchange interaction inGa1â^'xMnxAsdiluted magnetic semiconductors. Physical Review B, 2005, 72, .	1.1	13
165	Electronic transport properties of ascorbic acid and nicotinamide adsorbed on single-walled carbon nanotubes. Chemical Physics Letters, 2011, 506, 233-238.	1.2	13
166	Tuning the thermoelectric properties of a single-molecule junction by mechanical stretching. Physical Chemistry Chemical Physics, 2015, 17, 5386-5392.	1.3	13
167	Unveiling the dopant segregation effect at hematite interfaces. Applied Physics Letters, 2021, 118, .	1.5	13
168	Jacutingaite-family: A class of topological materials. Physical Review B, 2020, 102, .	1.1	13
169	Molecular cluster model of covalent semiconductors. Journal of Physics C: Solid State Physics, 1978, 11, L175-L177.	1.5	12
170	Comment on â€œContaminants in Suspended Gold Chains: AnAbÂInitioMolecular Dynamics Studyâ€• Physical Review Letters, 2005, 95, 169601; author reply 169602.	2.9	12
171	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
172	Graphene on amorphous HfO2surface: Anab initioinvestigation. Physical Review B, 2013, 87, .	1.1	12
173	Theoretical Study of the Siâ€A Centre. Physica Status Solidi (B): Basic Research, 1980, 98, K109.	0.7	11
174	Defect complexes in GaAs:â€ƒFirst-principles calculations. Physical Review B, 1997, 56, 13073-13076.	1.1	11
175	Vacancy-like defects in a-Si: a first principles study. Journal of Non-Crystalline Solids, 2004, 338-340, 400-402.	1.5	11
176	Interfaces between buckling phases in silicene:Ab initiodensity functional theory calculations. Physical Review B, 2013, 88, .	1.1	11
177	Valley Hall effect in silicene and hydrogenated silicene ruled by grain boundaries: Anab initioinvestigation. Physical Review B, 2015, 91, .	1.1	11
178	Electronic transport properties of MoS2 nanoribbons embedded in butadiene solvent. Physical Chemistry Chemical Physics, 2019, 21, 11359-11366.	1.3	11
179	Dual topological insulator device with disorder robustness. Physical Review B, 2020, 102, .	1.1	11
180	Study of the muffin-tin approximation in the multiple-scattering method. International Journal of Quantum Chemistry, 1979, 16, 1021-1031.	1.0	10

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181	Germanium negative-Ucenter in GaAs. Physical Review B, 1996, 53, 1315-1321.	1.1	10
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