Adalberto Fazzio

List of Publications by Citations

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	Electronic and transport properties of boron-doped graphene nanoribbons. *Physical Review Letters*, **2007**, 98, 196803	7.4	502
304	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
303	Switching a normal insulator into a topological insulator via electric field with application to phosphorene. *Nano Letters*, **2015**, 15, 1222-8	11.5	343
302	Many-electron multiplet effects in the spectra of 3d impurities in heteropolar semiconductors. *Physical Review B*, **1984**, 30, 3430-3455	3.3	233
301	A universal trend in the binding energies of deep impurities in semiconductors. *Applied Physics Letters*, **1984**, 45, 671-673	3.4	229
300	Ab initio calculations for a hypothetical material: Silicon nanotubes. *Physical Review B*, **2000**, 61, 9994-9996	3.3	209
299	From DFT to machine learning: recent approaches to materials science– review. *JPhys Materials*, **2019**, 2, 032001	4.2	206
298	How do gold nanowires break?. *Physical Review Letters*, **2001**, 87, 256102	7.4	191
297	Divacancies in graphene and carbon nanotubes. *Nano Letters*, **2007**, 7, 2459-62	11.5	151
296	Theoretical study of native defects in BN nanotubes. *Physical Review B*, **2003**, 67,	3.3	143
295	Electronic, structural, and transport properties of Ni-doped graphene nanoribbons. *Physical Review B*, **2009**, 79,	3.3	130
294	Structural properties of amorphous silicon nitride. *Physical Review B*, **1998**, 58, 8323-8328	3.3	127
293	Phenomenological band structure model of magnetic coupling in semiconductors. *Solid State Communications*, **2006**, 138, 353-358	1.6	117
292	Comparative study of defect energetics in HfO2 and SiO2. *Applied Physics Letters*, **2004**, 84, 1492-1494	3.4	102
291	Theoretical study of the formation, evolution, and breaking of gold nanowires. *Physical Review B*, **2004**, 69,	3.3	101
290	Electronic and structural properties of silicon-doped carbon nanotubes. *Physical Review B*, **2001**, 64,	3.3	98
289	Adsorption of CO and NO molecules on carbon doped boron nitride nanotubes. *Solid State Communications*, **2007**, 142, 49-53	1.6	96

288	Designing real nanotube-based gas sensors. *Physical Review Letters*, **2008**, 100, 176803	7.4	95
287	sigma- and pi-defects at graphene nanoribbon edges: building spin filters. *Nano Letters*, **2008**, 8, 2293-8	11.5	94
286	Ab initio study of an iron atom interacting with single-wall carbon nanotubes. *Physical Review B*, **2003**, 67,	3.3	94
285	Origin of FM ordering in pristine micro- and nanostructured ZnO. *Nano Letters*, **2010**, 10, 1383-6	11.5	92
284	Hydrogen adsorption on carbon-doped boron nitride nanotube. *Journal of Physical Chemistry B*, **2006**, 110, 21184-8	3.4	89
283	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
282	Electronic and Magnetic Properties of Ti and Fe on Graphene. *Journal of Physical Chemistry C*, **2008**, 112, 9163-9167	3.8	83
281	Stability investigation and thermal behavior of a hypothetical silicon nanotube. *Computational and Theoretical Chemistry*, **2001**, 539, 101-106		83
280	Hydrogen adsorption on boron doped graphene: an ab initio study. *Nanotechnology*, **2008**, 19, 155708	3.4	80
279	Directional dependence of the electronic and transport properties of 2D borophene and borophane. *Physical Chemistry Chemical Physics*, **2016**, 18, 25491-25496	3.6	77
278	Hydrogen role on the properties of amorphous silicon nitride. *Journal of Applied Physics*, **1999**, 86, 1843-1847	2.5	73
277	Vacancy formation process in carbon nanotubes: first-principles approach. *Nano Letters*, **2005**, 5, 197-200	11.5	72
276	Microscopic picture of the single vacancy in germanium. *Physical Review B*, **2000**, 61, R2401-R2404	3.3	72
275	Effect of impurities in the large Au-Au distances in gold nanowires. *Physical Review Letters*, **2003**, 90, 036101	7.4	69
274	Formation energy of native defects in BN nanotubes: anab initiostudy. *Nanotechnology*, **2005**, 16, 827-831	3.4	69
273	Surface magnetization in non-doped ZnO nanostructures. *Applied Physics Letters*, **2009**, 94, 162503	3.4	67
272	Electronic structure of copper, silver, and gold impurities in silicon. *Physical Review B*, **1985**, 32, 934-954	3.3	66
271	Electronic structure of Cu, Ni, Co, and Fe substitutional impurities in gallium arsenide. *Physical Review B*, **1980**, 21, 4710-4720	3.3	64

270	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
269	Functionalization of carbon nanotubes through the chemical binding of atoms and molecules. *Physical Review B*, **2003**, 67,	3.3	63
268	Oxygen clamps in gold nanowires. *Physical Review Letters*, **2006**, 96, 016104	7.4	60
267	Barrier-free substitutional doping of graphene sheets with boron atoms: Ab initio calculations. *Physical Review B*, **2009**, 79,	3.3	57
266	Ab initio determination of the atomistic structure of SixGe1⊠ alloy. *Physical Review B*, **2001**, 64,	3.3	56
265	Ferromagnetic coupling in a Co-doped graphenelike ZnO sheet. *Physical Review B*, **2010**, 81,	3.3	54
264	Edge effects in bilayer graphene nanoribbons: Ab initio total-energy density functional theory calculations. *Physical Review B*, **2009**, 79,	3.3	54
263	Confinement and surface effects in B and P doping of silicon nanowires. *Nano Letters*, **2008**, 8, 1866-71	11.5	53
262	Density functional theory method for non-equilibrium charge transport calculations: TRANSAMPA. *Brazilian Journal of Physics*, **2006**, 36, 799-807	1.2	51
261	Formation of atomic carbon chains from graphene nanoribbons. *Physical Review B*, **2010**, 81,	3.3	50
260	First-principles calculations of carbon nanotubes adsorbed on Si(001). *Physical Review Letters*, **2003**, 91, 166802	7.4	50
259	Self-interstitial defect in germanium. *Physical Review B*, **2000**, 62, 9903-9906	3.3	50
258	Anion-antisite-like defects in III-V compounds. *Physical Review Letters*, **1990**, 65, 2046-2049	7.4	48
257	The 2021 quantum materials roadmap. *JPhys Materials*, **2020**, 3, 042006	4.2	48
256	Two-dimensional van der Waals p-n junction of InSe/phosphorene. *Physical Review B*, **2017**, 95,	3.3	47
255	Multiple scattering-X⊠luster model of GaAs: electronic states of isolated vacancies and substitutional impurities. *Journal of Physics C: Solid State Physics*, **1979**, 12, 3469-3481		47
254	Quantum spin Hall effect on germanene nanorod embedded in completely hydrogenated germanene. *Physical Review B*, **2014**, 89,	3.3	46
253	Topological insulator Bi2Se3(111) surface doped with transition metals: An ab initio investigation. *Physical Review B*, **2013**, 88,	3.3	46

252	Separation of one- and many-electron effects in the excitation spectra of 3d impurities in semiconductors. *Physical Review B*, **1984**, 29, 5999-6002	3.3	46
251	Spin texture and magnetic anisotropy of Co impurities in Bi2Se3 topological insulators. *Physical Review B*, **2011**, 84,	3.3	45
250	Surface and Quantum Confinement Effects in ZnO Nanocrystals. *Journal of Physical Chemistry C*, **2010**, 114, 18293-18297	3.8	45
249	Doping of graphene adsorbed on the a-SiO2 surface. *Applied Physics Letters*, **2011**, 99, 163108	3.4	43
248	Exploring Two-Dimensional Materials Thermodynamic Stability via Machine Learning. *ACS Applied Materials & Interfaces*, **2020**, 12, 20149-20157	9.5	43
247	Theoretical investigation of a possible MnxSi1⊠ ferromagnetic semiconductor. *Physical Review B*, **2003**, 68,	3.3	42
246	Metal Chalcogenides Janus Monolayers for Efficient Hydrogen Generation by Photocatalytic Water Splitting. *ACS Applied Nano Materials*, **2019**, 2, 890-897	5.6	40
245	Amorphous HfO2 and Hf1⊠SixO via a melt-and-quench scheme using ab initio molecular dynamics. *Physical Review B*, **2008**, 77,	3.3	39
244	Stabilization of substitutional Mn in silicon-based semiconductors. *Physical Review B*, **2004**, 70,	3.3	38
243	Substitutional Si Doping in Deformed Carbon Nanotubes. *Nano Letters*, **2004**, 4, 975-977	11.5	38
242	Energetics and stability of vacancies in carbon nanotubes. *Solid State Communications*, **2011**, 151, 482-486	1.6	37
241	Si nanowires as sensors: choosing the right surface. *Nano Letters*, **2007**, 7, 1172-7	11.5	37
240	First-principles investigation of a⊠iNx:H. *Physical Review B*, **2002**, 65,	3.3	37
239	Stability and electronic confinement of free-standing InP nanowires: Ab initio calculations. *Physical Review B*, **2005**, 72,	3.3	35
238	Optical Transitions in Ruby across the Corundum to Rh2O3 (II) Phase Transformation. *Physical Review Letters*, **1998**, 81, 3267-3270	7.4	35
237	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
236	Organic molecule assembled between carbon nanotubes: A highly efficient switch device. *Physical Review B*, **2009**, 79,	3.3	34
235	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

234	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
233	Orientational defects in ice Ih: an interpretation of electrical conductivity measurements. *Physical Review Letters*, **2006**, 96, 075501	7.4	34
232	Substrate-dependent electronic properties of an armchair carbon nanotube adsorbed on H□Si(001). *Applied Physics Letters*, **2005**, 86, 213111	3.4	33
231	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		33
230	Electronic and structural trends in small GaAs clusters. *Scripta Materialia*, **1998**, 10, 635-647		32
229	Transport properties of single vacancies in nanotubes. *Physical Review B*, **2008**, 77,	3.3	32
228	Bundling up carbon nanotubes through Wigner defects. *Nano Letters*, **2005**, 5, 1045-9	11.5	32
227	Electronic and magnetic properties of iron chains on carbon nanotubes. *Microelectronics Journal*, **2003**, 34, 481-484	1.8	32
226	Theoretical investigation of the electrical and optical activity of vanadium in GaAs. *Physical Review B*, **1986**, 33, 7102-7109	3.3	32
225	Short linear atomic chains in copper nanowires. *Nanotechnology*, **2007**, 18, 145701	3.4	30
224	Vacancy-mediated diffusion in disordered alloys: Ge self-diffusion in Si1□Gex. *Physical Review B*, **2002**, 65,	3.3	30
223	Bilayer graphene dual-gate nanodevice: An ab initio simulation. *Physical Review B*, **2011**, 84,	3.3	29
222	First-principles study of the adsorption of atomic and molecular hydrogen on BC2N nanotubes. *Physical Review B*, **2008**, 77,	3.3	29
221	Temperature and quantum effects in the stability of pure and doped gold nanowires. *Physical Review Letters*, **2008**, 100, 056104	7.4	29
220	Oxidation at the Si/SiO2 interface: influence of the spin degree of freedom. *Physical Review Letters*, **2003**, 90, 016103	7.4	29
219	O2 diffusion in SiO2: triplet versus singlet. *Physical Review Letters*, **2001**, 87, 155901	7.4	29
218	Point defect interactions with extended defects in semiconductors. *Physical Review B*, **1999**, 60, 4711-4714	3.3	29
217	Ambipolar Resistive Switching in an Ultrathin Surface-Supported Metal-Organic Framework Vertical Heterojunction. *Nano Letters*, **2020**, 20, 1080-1088	11.5	29

216	Theoretical investigations of Ge nanowires grown along the [110] and [111] directions. *Nanotechnology*, **2007**, 18, 295706	3.4	28
215	Disorder-based graphene spintronics. *Nanotechnology*, **2010**, 21, 345202	3.4	27
214	Electronic and magnetic properties of Mn-doped InP nanowires from first principles. *Physical Review B*, **2006**, 73,	3.3	27
213	Oxidation of free-standing and supported borophene. *2D Materials*, **2017**, 4, 025025	5.9	26
212	Theoretical studies of native defects in cubic boron nitride. *Physical Review B*, **1997**, 56, 3556-3559	3.3	26
211	Adatoms in graphene as a source of current polarization: Role of the local magnetic moment. *Physical Review B*, **2011**, 84,	3.3	25
210	Role played by N and N-N impurities in type-IV semiconductors. *Physical Review B*, **1993**, 48, 17806-17810	3.3	25
209	Topological phases in triangular lattices of Ru adsorbed on graphene: Ab initio calculations. *Physical Review B*, **2014**, 89,	3.3	23
208	Energetics and structural properties of adsorbed atoms and molecules on silicon-doped carbon nanotubes. *Materials Characterization*, **2003**, 50, 183-187	3.9	23
207	Vertical twinning of the Dirac cone at the interface between topological insulators and semiconductors. *Nature Communications*, **2015**, 6, 7630	17.4	22
206	Confinement effects and why carbon nanotube bundles can work as gas sensors. *Nanoscale*, **2013**, 5, 2798-803	7.7	22
205	First principles study of titanium-coated carbon nanotubes as sensors for carbon monoxide molecules. *Surface Science*, **2007**, 601, 4102-4104	1.8	22
204	Titanium monomers and wires adsorbed on carbon nanotubes: a first principles study. *Nanotechnology*, **2006**, 17, 1154-9	3.4	22
203	Dislocation core properties in semiconductors. *Solid State Communications*, **2001**, 118, 651-655	1.6	22
202	Quantum spin Hall effect in a disordered hexagonal SixGe1⊠ alloy. *Physical Review B*, **2013**, 88,	3.3	21
201	Structural and electronic properties of silicon nitride materials. *International Journal of Quantum Chemistry*, **1998**, 70, 973-980	2.1	21
200	Structure and energetics of molecular point defects in ice Ih. *Physical Review Letters*, **2006**, 97, 155501	7.4	21
199	Symmetry controlled spin polarized conductance in au nanowires. *Journal of the American Chemical Society*, **2008**, 130, 9897-903	16.4	20

198	Diffusion-reaction mechanisms of nitriding species in SiO2. *Physical Review B*, **2004**, 70,	3.3	20
197	Structural order and clustering in annealed SiC and SiC:H. *Physical Review B*, **2002**, 65,	3.3	20
196	Toward Realistic Amorphous Topological Insulators. *Nano Letters*, **2019**, 19, 8941-8946	11.5	19
195	Topological states ruled by stacking faults in Bi2Se3 and Bi2Te3. *Journal of Applied Physics*, **2013**, 113, 023705	2.5	19
194	Fe and Mn atoms interacting with carbon nanotubes. *Physica B: Condensed Matter*, **2003**, 340-342, 982-985	2.8	19
193	Realistic calculations of carbon-based disordered systems. *Journal Physics D: Applied Physics*, **2010**, 43, 374002	3	18
192	Breaking of gold nanowires. *Computational Materials Science*, **2004**, 30, 73-76	3.2	18
191	Theoretical investigation of the pressure induced cubic-diamond-tin phase transition in the Si0.5Ge0.5. *Solid State Communications*, **2001**, 120, 369-373	1.6	18
190	Effects of extended defects on the properties of intrinsic and extrinsic point defects in silicon. *Physica B: Condensed Matter*, **1999**, 273-274, 473-475	2.8	18
189	Theoretical model of the Au-Fe complex in silicon. *Physical Review B*, **1985**, 32, 8085-8091	3.3	18
188	Simulations and Materials Chemistry in the Age of Big Data. *Journal of Chemical Information and Modeling*, **2020**, 60, 452-459	6.1	18
187	Quantum confinement effects on Mn-doped InAs nanocrystals: A first-principles study. *Physical Review B*, **2008**, 78,	3.3	17
186	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
185	Electronic and structural properties of vacancy and self-interstitial defects in germanium. *Physica B: Condensed Matter*, **1999**, 273-274, 575-578	2.8	17
184	Directional Control of the Electronic and Transport Properties of Graphynes. *Journal of Physical Chemistry C*, **2014**, 118, 18793-18798	3.8	16
183	IxV curves of boron and nitrogen doping zigzag graphene nanoribbons. *International Journal of Quantum Chemistry*, **2011**, 111, 1379-1386	2.1	16
182	Gold nanowires and the effect of impurities. *Nanoscale Research Letters*, **2006**, 1, 91-98	5	16
181	Structural, electronic, and magnetic properties of Mn-doped Ge nanowires by ab initio calculations. *Physical Review B*, **2007**, 75,	3.3	16

180	Formation and structural properties of the amorphous-crystal interface in a nanocrystalline system. *Physical Review B*, **2001**, 64,	3.3	16
179	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
178	Spin caloritronics in graphene with Mn. *Applied Physics Letters*, **2014**, 104, 072412	3.4	15
177	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
176	Anab initiostudy of manganese atoms and wires interacting with carbon nanotubes. *Journal of Physics Condensed Matter*, **2004**, 16, 3647-3661	1.8	15
175	Stability and electronic properties of carbon nanotubes adsorbed on Si(0 0 1). *Surface Science*, **2004** , 566-568, 728-732	1.8	15
174	First principles study of the ferromagnetism in Ga1−xMnxAs semiconductors. *Journal of Physics Condensed Matter*, **2004**, 16, 8243-8250	1.8	15
173	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
172	Mn dimers on graphene nanoribbons: An ab initio study. *Journal of Applied Physics*, **2011**, 109, 053715	2.5	14
171	Ab initio calculations of vacancies in SixGe1−x. *Applied Physics Letters*, **2002**, 81, 3383-3385	3.4	14
170	Dislocation core reconstruction in zinc-blende semiconductors. *Journal of Physics Condensed Matter* , **2000**, 12, 10039-10044	1.8	14
169	Zeeman-type spin splitting in nonmagnetic three-dimensional compounds. *Npj Quantum Materials*, **2019**, 4,	5	13
168	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
167	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
166	Spin filtering and disorder-induced magnetoresistance in carbon nanotubes: Ab initio calculations. *Physical Review B*, **2011**, 84,	3.3	13
165	Interaction of As impurities with 30°partial dislocations in Si: An ab initio investigation. *Journal of Applied Physics*, **2002**, 91, 5892-5895	2.5	13
164	Disorder and the effective Mn–Mn exchange interaction in Ga1−xMnxAs diluted magnetic semiconductors. *Physical Review B*, **2005**, 72,	3.3	13
163	Many-electron treatment of the off-center substitutional O in Si. *Physical Review B*, **1986**, 33, 4432-4435	3.3	13

162	Multiple-scattering X□molecular-cluster model of complex defects in semiconductors: Application to Si:P2 and Si:P2+ systems. *Physical Review B*, **1982**, 25, 2603-2610	3.3	13
161	Electronic structure of neutral and negatively charged gallium vacancies in GaP. *Journal of Physics C: Solid State Physics*, **1982**, 15, L1-L3		13
160	Splitting of the zero-energy edge states in bilayer graphene. *Physical Review B*, **2010**, 81,	3.3	12
159	Molecular cluster model of covalent semiconductors. *Journal of Physics C: Solid State Physics*, **1978**, 11, L175-L177		12
158	Tuning the thermoelectric properties of a single-molecule junction by mechanical stretching. *Physical Chemistry Chemical Physics*, **2015**, 17, 5386-92	3.6	11
157	Unconventional spin texture in a noncentrosymmetric quantum spin Hall insulator. *Physical Review B*, **2016**, 94,	3.3	11
156	Size- effect induced high thermoelectric figure of merit in PbSe and PbTe nanowires. *Physical Chemistry Chemical Physics*, **2014**, 16, 8114-8	3.6	11
155	Graphene on amorphous HfO2 surface: An ab initio investigation. *Physical Review B*, **2013**, 87,	3.3	11
154	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
153	Theoretical Study of the Si-A Centre. *Physica Status Solidi (B): Basic Research*, **1980**, 98, K109-K111	1.3	11
152	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
151	Graphene nanoribbon intercalated with hexagonal boron nitride: Electronic transport properties from ab initio calculations. *Solid State Communications*, **2013**, 173, 24-29	1.6	10
150	Interfaces between buckling phases in silicene: Ab initio density functional theory calculations. *Physical Review B*, **2013**, 88,	3.3	10
149	Electronic transport properties of ascorbic acid and nicotinamide adsorbed on single-walled carbon nanotubes. *Chemical Physics Letters*, **2011**, 506, 233-238	2.5	10
148	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
147	Defect complexes in GaAs: First-principles calculations. *Physical Review B*, **1997**, 56, 13073-13076	3.3	10
146	Stacking fault effects in pure and n-type doped GaAs. *Applied Physics Letters*, **2001**, 78, 907-909	3.4	10
145	Initial stages of Ge growth on Si(100): ad-atoms, ad-dimers, and ad-trimers. *Physica B: Condensed Matter*, **1999**, 273-274, 589-592	2.8	10

144	Germanium negative-U center in GaAs. *Physical Review B*, **1996**, 53, 1315-1321	3.3	10
143	Adsorption of 3d, 4d, and 5d transition metal atoms on □Borophene. *Journal of Physics Condensed Matter*, **2017**, 29, 305302	1.8	9
142	Theoretical and Experimental Investigation of 2D Hematite. *Journal of Physical Chemistry C*, **2019**, 123, 16359-16365	3.8	9
141	Decreasing Nanocrystal Structural Disorder by Ligand Exchange: An Experimental and Theoretical Analysis. *Journal of Physical Chemistry Letters*, **2019**, 10, 1471-1476	6.4	9
140	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
139	Topological phase transitions of (BixSb1-x)2Se3 alloys by density functional theory. *Journal of Physics Condensed Matter*, **2015**, 27, 255501	1.8	9
138	First-principles study of HgTe/CdTe heterostructures under perturbations preserving time-reversal symmetry. *Physical Review B*, **2014**, 90,	3.3	9
137	Quantum confinement and spin-orbit interactions in PbSe and PbTe nanowires: First-principles calculation. *Physical Review B*, **2011**, 84,	3.3	9
136	Theoretical investigation of a Mn-doped Si□e heterostructure. *Physical Review B*, **2007**, 75,	3.3	9
135	Adsorption of Mn atoms on the Si(1 0 0) surface. *Surface Science*, **2004**, 566-568, 688-692	1.8	9
134	Electronic structure and origin of ferromagnetism in Ga1□MnxAs semiconductors. *Physica B: Condensed Matter*, **2003**, 340-342, 874-877	2.8	9
133	Vacancy-like defects in a-Si: a first principles study. *Journal of Non-Crystalline Solids*, **2004**, 338-340, 400-402	3.2	9
132	Electronic structure calculation of V2+O2 complexes in silicon. *Solid State Communications*, **1984**, 49, 537-539	1.6	9
131	Study of the muffin-tin approximation in the multiple-scattering method. *International Journal of Quantum Chemistry*, **1979**, 16, 1021-1031	2.1	9
130	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
129	Stacking-dependent transport properties in few-layers graphene. *Solid State Communications*, **2017**, 250, 70-74	1.6	8
128	Electronic transport in patterned graphene nanoroads. *Nanotechnology*, **2013**, 24, 495201	3.4	8
127	Valley Hall effect in silicene and hydrogenated silicene ruled by grain boundaries: An ab initio investigation. *Physical Review B*, **2015**, 91,	3.3	8

126	Mimicking nanoribbon behavior using a graphene layer on SiC. *Physical Review B*, **2010**, 82,	3.3	8
125	C59Si on the monohydride Si(100):H-(2 x 1) surface. *Journal of Physical Chemistry B*, **2006**, 110, 10849-54	3.4	8
124	Carbon in SixGe1−x: An ab initio investigation. *Physical Review B*, **2004**, 69,	3.3	8
123	Theoretical and experimental studies of the atomic structure of oxygen-rich amorphous silicon oxynitride films. *Physical Review B*, **2003**, 68,	3.3	8
122	Adsorption of monomers on semiconductors and the importance of surface degrees of freedom. *Physical Review B*, **2001**, 63,	3.3	8
121	Ab Initio Study of N Impurity in Amorphous Germanium. *Physical Review Letters*, **1996**, 77, 546-549	7.4	8
120	Silicene-Based FET for Logical Technology. *IEEE Electron Device Letters*, **2018**, 39, 1258-1261	4.4	7
119	Simple implementation of complex functionals: scaled self-consistency. *Journal of Chemical Physics*, **2007**, 126, 144107	3.9	7
118	Ab initio calculation of electronic properties of periodically Si- delta -doped GaAs. *Physical Review B*, **1995**, 51, 7898-7900	3.3	7
117	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
116	Pair Distribution Function Obtained from Electron Diffraction: An Advanced Real-Space Structural Characterization Tool. *Matter*, **2021**, 4, 441-460	12.7	7
115	Machine learning for materials discovery: Two-dimensional topological insulators. *Applied Physics Reviews*, **2021**, 8, 031409	17.3	7
114	On the nature of the solvated electron in ice Ih. *Physical Chemistry Chemical Physics*, **2016**, 18, 4652-8	3.6	6
113	Tight-binding model for the band dispersion in rhombohedral topological insulators over the whole Brillouin zone. *Physical Review B*, **2018**, 98,	3.3	6
112	Novel III-Te-graphene van der Waals heterojunctions for optoelectronic devices. *RSC Advances*, **2017**, 7, 32383-32390	3.7	6
111	First-principles study of group III impurity doped PbSe: Bulk and nanowire. *Physical Review B*, **2013**, 87,	3.3	6
110	EL2-like defects in InP nanowires: An ab initio total energy investigation. *Physical Review B*, **2007**, 75,	3.3	6
109	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

108	Effect of impurities on the breaking of Au nanowires. *Surface Science*, **2004**, 566-568, 367-371	1.8	6
107	Native defects in germanium. *Physica B: Condensed Matter*, **2001**, 302-303, 364-368	2.8	6
106	[PIn](n) antisite clustering in InP. *Physical Review B*, **1999**, 60, 16475-16478	3.3	6
105	Carbon doping of GaAs: Compensation effects. *Applied Physics Letters*, **1995**, 66, 2715-2717	3.4	6
104	Studies of the local reactivity of surfaces using chemical based principles. *Surface Science*, **1994**, 313, 41-51	1.8	6
103	Correlation Effects in Native Defects in GaAs. *Materials Science Forum*, **1991**, 38-41, 119-124	0.4	6
102	Theory of interstitial transition atoms in GaAs. *Physical Review B*, **1987**, 36, 7542-7548	3.3	6
101	A molecular cluster study of complex defects in Si: The divacancy and the E center. *Physica B: Physics of Condensed Matter & C: Atomic, Molecular and Plasma Physics, Optics*, **1983**, 116, 90-94		6
100	Electronic structure of oxygen in silicon. *Physica B: Physics of Condensed Matter & C: Atomic, Molecular and Plasma Physics, Optics*, **1983**, 116, 106-111		6
99	Electronic structure of a single neutral ideal phosphorus vacancy in GaP. *Journal of Physics C: Solid State Physics*, **1984**, 17, 3423-3428		6
98	Many-electron multiplet effects in the optical spectra of NiO, CoO and MnO. *Solid State Communications*, **1984**, 52, 265-269	1.6	6
97	Electronic structure of oxygen-doped gallium arsenide. *Journal of Physics C: Solid State Physics*, **1979**, 12, L831-L834		6
96	Dual topological insulator device with disorder robustness. *Physical Review B*, **2020**, 102,	3.3	6
95	Inverse design of compounds that have simultaneously ferroelectric and Rashba cofunctionality. *Physical Review B*, **2020**, 102,	3.3	6
94	Structural and electronic properties of realistic two-dimensional amorphous topological insulators. *2D Materials*, **2021**, 8, 025032	5.9	6
93	Electronic transport properties of MoS nanoribbons embedded in butadiene solvent. *Physical Chemistry Chemical Physics*, **2019**, 21, 11359-11366	3.6	5
92	Carrier-mediated magnetism in transition metal doped Bi_2Se_3 topological insulator. *Journal of Physics Condensed Matter*, **2013**, 25, 445003	1.8	5
91	Piezomagnetic behavior of Co-doped ZnO nanoribbons. *Physical Review B*, **2011**, 84,	3.3	5

90	Carbon nanotube adsorbed on hydrogenated Si(001) surfaces. *Applied Surface Science*, **2005**, 244, 124-128	3.7	5
89	Oxygen-induced atomic desorptions in oxynitrides: Density functional calculations. *Physical Review B*, **2005**, 72,	3.3	5
88	Two-atom structures of Ge on Si(100): dimers versus adatom pairs. *Physical Review Letters*, **2001**, 87, 036104	7.4	5
87	Arsenic segregation, pairing and mobility on the cores of partial dislocations in silicon. *Journal of Physics Condensed Matter*, **2002**, 14, 12761-12765	1.8	5
86	Defect-molecule parameters for the divacancy in silicon. *Solid State Communications*, **1985**, 53, 841-844	1.6	5
85	Electronic structure calculation of Mn-doped GaAs. *Solid State Communications*, **1982**, 44, 369-372	1.6	5
84	Controlling Topological States in Topological/Normal Insulator Heterostructures. *ACS Omega*, **2018**, 3, 15900-15906	3.9	5
83	Semiclassical transport properties of IrGa: a promising thermoelectric material. *Journal of Physics Condensed Matter*, **2018**, 30, 085701	1.8	4
82	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
81	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
80	Hf defects in c-Si and their importance for the HfO2/Si interface: Density-functional calculations. *Physical Review B*, **2007**, 75,	3.3	4
79	Silicon adsorption in defective carbon nanotubes: a first principles study. *Nanotechnology*, **2006**, 17, 4088-91	3.4	4
78	Theoretical investigation of extended defects and their interactions with vacancies in SixGe1-x. *Physical Review B*, **2003**, 67,	3.3	4
77	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
76	Segregation of dopant atoms on extended defects in semiconductors. *Physica B: Condensed Matter*, **2001**, 302-303, 403-407	2.8	4
75	The effect of a stacking fault on the electronic properties of dopants in gallium arsenide. *Journal of Physics Condensed Matter*, **2000**, 12, 10235-10239	1.8	4
74	Concerted-exchange mechanism for antistructure pair defects in GaAs. *Solid State Communications*, **1999**, 110, 457-461	1.6	4
73	CLUSTER CALCULATION OF THE ELECTRONIC STRUCTURE OF K3C60. *Modern Physics Letters B*, **1995**, 09, 95-101	1.6	4

72	Intra-d excitations: Comparison between approaches for impurities in semiconductors. *Physical Review B*, **1988**, 37, 4770-4773	3.3	4
71	Theoretical Study of Single Vacancies in GaSb. *Physica Status Solidi (B): Basic Research*, **1981**, 105, 339-345	1.3	4
70	Theoretical study of the F2molecule using the variational cellular method. *Journal of Physics B: Atomic and Molecular Physics*, **1981**, 14, L533-L535		4
69	Defect centers in a-SiNx: electronic and structural properties. *Brazilian Journal of Physics*, **2002**, 32, 436-438	1.2	4
68	Unveiling the dopant segregation effect at hematite interfaces. *Applied Physics Letters*, **2021**, 118, 201602	3.4	4
67	Topological states of nanoscale Bi2Se3 interfaced with AlN. *Applied Physics Letters*, **2016**, 109, 131601	3.4	4
66	Structural evolution and the role of native defects in subnanometer MoS nanowires. *Physical Review B*, **2019**, 100,	3.3	4
65	Oxidation of Ni13 clusters. *International Journal of Quantum Chemistry*, **2019**, 119, e25874	2.1	4
64	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
63	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
62	Dynamic covalent bond from first principles: Diarylbibenzofuranone structural, electronic, and oxidation studies. *Journal of Computational Chemistry*, **2017**, 38, 2675-2679	3.5	3
61	Initial stages of Ge and Si growth near SB monoatomic steps on Si(100). *Physical Review B*, **2004**, 70,	3.3	3
60	The energetics of dislocation cores in semiconductors and their role on dislocation mobility. *Physica B: Condensed Matter*, **2001**, 302-303, 398-402	2.8	3
59	Intrinsic doping in InP: ab initio calculations of PIn antisites. *Physica B: Condensed Matter*, **1999**, 273-274, 831-834	2.8	3
58	Structural and electronic studies of Ga3As3, Ga4As3, and Ga3As4. *International Journal of Quantum Chemistry*, **1994**, 52, 571-577	2.1	3
57	Ab Initio Cluster Calculation of Hyperfine Interactions and Total-Energy Surfaces for N in Diamond, Silicon and Germanium. *Materials Science Forum*, **1992**, 83-87, 463-468	0.4	3
56	Anion Antisite defects in GaAs: As and Sb. *International Journal of Quantum Chemistry*, **1990**, 38, 563-567	2.1	3
55	Jacutingaite-family: A class of topological materials. *Physical Review B*, **2020**, 102,	3.3	3

54	Room-Temperature Negative Differential Resistance in Surface-Supported Metal-Organic Framework Vertical Heterojunctions. *Small*, **2021**, 17, e2101475	11	3
53	Band gap tuning of layered III-Te materials. *Journal of Applied Physics*, **2018**, 124, 045104	2.5	3
52	Mn-doped cubic BN as an atomiclike memory device: A density functional study. *Physical Review B*, **2010**, 81,	3.3	2
51	Electronic and structural properties of C59Si on the monohydride Si(100) surface. *International Journal of Quantum Chemistry*, **2005**, 103, 557-561	2.1	2
50	Many-electron effects on the structural properties of sp impurities in semiconductors. *Solid State Communications*, **1992**, 82, 83-87	1.6	2
49	Electronic states induced by a Ga vacancy in the GaAs1−xPx alloy. *International Journal of Quantum Chemistry*, **1993**, 48, 213-217	2.1	2
48	The Cr2+ luminescence in GaAs as a function of hydrostatic pressure. *Solid State Communications*, **1989**, 69, 461-463	1.6	2
47	Excitation and ionization of Mo and W in GaAs. *Physical Review B*, **1986**, 34, 2690-2694	3.3	2
46	Analysis of pseudo-Jahn-Teller instability: O, S, and N- in silicon. *Physical Review B*, **1987**, 35, 6450-6453	3.3	2
45	Electronic structure of GaP:O via the MS-Xα method. *Journal of Physics and Chemistry of Solids*, **1983**, 44, 349-351	3.9	2
44	Discovery of higher-order topological insulators using the spin Hall conductivity as a topology signature. *Npj Computational Materials*, **2021**, 7,	10.9	2
43	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
42	Distilling small volumes of crude oil. *Fuel*, **2021**, 285, 119072	7.1	2
41	Emergent quasiparticles in Euclidean tilings. *Nanoscale*, **2021**, 13, 5270-5274	7.7	2
40	Daphnia magna and mixture toxicity with nanomaterials □Current status and perspectives in data-driven risk prediction. *Nano Today*, **2022**, 43, 101430	17.9	2
39	Substrate-supported large-band-gap quantum spin Hall insulator based on III-V bismuth layers. *Physical Review B*, **2016**, 94,	3.3	1
38	Point defects in covalent semiconductors: A molecular cluster model. *International Journal of Quantum Chemistry*, **2009**, 16, 349-361	2.1	1
37	Ab initio studies of the Si1−xGex alloy and its intrinsic defects. *Computational Materials Science*, **2001**, 22, 62-66	3.2	1

36	Theoretical study of defect complexes related with antisites in GaAs. *Radiation Effects and Defects in Solids*, **1998**, 146, 65-70	0.9	1
35	Metal□nsulator transition in fullerides: K3C60 versus Na3C60. *International Journal of Quantum Chemistry*, **1995**, 56, 217-219	2.1	1
34	Impurity states in the narrow band-gap semiconductor n-type InSb. *Solid State Communications*, **1996**, 99, 295-297	1.6	1
33	Theoretical investigation of the electronic structure and absorption spectra of carbon cluster nanotubes. *Scripta Materialia*, **1994**, 4, 11-18		1
32	Theoretical investigation of the optical spectra of superconducting YBa2Cu3O7. *Solid State Communications*, **1991**, 78, 91-93	1.6	1
31	Electronic and structural properties of N and N2 in type-IV semiconductors. *International Journal of Quantum Chemistry*, **1992**, 44, 667-672	2.1	1
30	On the possibility of negative U systems for transition metals impurities in semiconductors. *International Journal of Quantum Chemistry*, **1987**, 32, 73-78	2.1	1
29	Charge stabilization of Cr at interstitial sites in GaAs. *Solid State Communications*, **1988**, 66, 1031-1033	1.6	1
28	Multiple scattering mass operator method for molecular orbital calculations. *International Journal of Quantum Chemistry*, **1980**, 18, 1165-1173	2.1	1
27	A simple way of eliminating the exchange parameter in the multiple scattering method. *Solid State Communications*, **1980**, 35, 329-331	1.6	1
26	Considera□s sobre o Programa Brasileiro de Nanotecnologia. *Ci□ncia E Cultura*, **2013**, 65, 23-27	0.3	1
25	Recent Advances in Immunosafety and Nanoinformatics of Two-Dimensional Materials Applied to Nano-imaging. *Frontiers in Immunology*, **2021**, 12, 689519	8.4	1
24	Bandgap evolution in nanographene assemblies. *Physical Chemistry Chemical Physics*, **2021**, 23, 11501-11506	3.6	1
23	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
22	At the Verge of Topology: Vacancy-Driven Quantum Spin Hall in Trivial Insulators. *Nano Letters*, **2021**, 21, 9398-9402	11.5	0
21	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
20	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
19	Conformational analysis of tannic acid: Environment effects in electronic and reactivity properties. *Journal of Chemical Physics*, **2021**, 154, 224102	3.9	0

18	Nanoporous ZnO: Structural and electronic study under biaxial strain. *Computational Materials Science*, **2018**, 149, 91-97	3.2
17	Nanodots of transition metal dichalcogenides embedded in MoS and MoSe: first-principles calculations. *Physical Chemistry Chemical Physics*, **2017**, 19, 26240-26247	3.6
16	Light emission and current rectification in a molecular device: Experiment and theory. *Journal of Applied Physics*, **2012**, 112, 113108	2.5
15	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
14	MS-X□Treatment for native defects in GaSb. *International Journal of Quantum Chemistry*, **2009**, 20, 457-457	2.1
13	Native defects and transition metal impurities at interstitial sites in gaas. *International Journal of Quantum Chemistry*, **2009**, 36, 677-685	2.1
12	Metal-semiconductor transition in cerium hydrides. *International Journal of Quantum Chemistry*, **2009**, 36, 709-716	2.1
11	Theoretical investigation of Hf and Zr defects in c-Ge. *Journal of Physics Condensed Matter*, **2009**, 21, 012206	1.8
10	Electronic and structural properties of defects in c-BN. *International Journal of Quantum Chemistry*, **1997**, 65, 941-946	2.1
9	Ab initio study of group V elements in amorphous silicon. *Journal of Non-Crystalline Solids*, **1998**, 227-230, 372-375	3.9
8	Ab initio calculations on the compensation mechanisms in InP. *Solid State Communications*, **2001**, 117, 353-355	1.6
7	Influence of surface degrees of freedom on the adsorption of Ge ad-atoms on Si(1 0 0). *Computational Materials Science*, **2001**, 22, 19-23	3.2
6	Electronic structure of periodically Si-□doped GaAs. *International Journal of Quantum Chemistry*, **1995**, 56, 203-206	2.1
5	Investigation of the many-particle spectrum of superconductor YBa2Cu3O7. *Bulletin of Materials Science*, **1991**, 14, 989-992	1.7
4	Many-electron treatment for chalcogen complexes in silicon. *Semiconductor Science and Technology* , **1990**, 5, 196-199	1.8
3	Progress in the study of transition metal impurities in III-V and II-VI materials. *International Journal of Quantum Chemistry*, **1987**, 32, 65-72	2.1
2	A new model for the Si-A center **1983**, 102-107	
1	High-throughput inverse design and Bayesian optimization of functionalities: spin splitting in two-dimensional compounds.. *Scientific Data*, **2022**, 9, 195	8.2