

# Alessandro Pecchia

## List of Publications by Year in descending order

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338  
papers

10,962  
citations

29994

54  
h-index

45213

90  
g-index

342  
all docs

342  
docs citations

342  
times ranked

12993  
citing authors

#	ARTICLE	IF	CITATIONS
1	DFTB+, a software package for efficient approximate density functional theory based atomistic simulations. Journal of Chemical Physics, 2020, 152, 124101.	1.2	589
2	Titanium-carbide MXenes for work function and interface engineering in perovskite solar cells. Nature Materials, 2019, 18, 1228-1234.	13.3	418
3	Efficiency Drop in Green Emitting Diodes: The Role of Random Alloy Fluctuations. Physical Review Letters, 2016, 116, 027401.	2.9	127
4	Charge transport in disordered graphene-based low dimensional materials. Nano Research, 2008, 1, 361-394.	5.8	319
5	Atomistic theory of transport in organic and inorganic nanostructures. Reports on Progress in Physics, 2004, 67, 1497-1561.	8.1	279
6	Application of silicene, germanene and stanene for Na or Li ion storage: A theoretical investigation. Electrochimica Acta, 2016, 213, 865-870.	2.6	245
7	Contact Dependence of Carrier Injection in Carbon Nanotubes: An Ab Initio Study. Physical Review Letters, 2006, 96, 076802.	2.9	194
8	Tuning the conductance of a molecular switch. Nature Nanotechnology, 2007, 2, 176-179.	15.6	188
9	Chirality-Dependent Electron Spin Filtering by Molecular Monolayers of Helicenes. Journal of Physical Chemistry Letters, 2018, 9, 2025-2030.	2.1	154
10	Efficient Calculation of Charge-Transfer Matrix Elements for Hole Transfer in DNA. Journal of Physical Chemistry B, 2008, 112, 7937-7947.	1.2	150
11	Decacene: On-Surface Generation. Angewandte Chemie - International Edition, 2017, 56, 11945-11948.	7.2	146
12	Coordination Polymer Framework Based On-Chip Micro-Supercapacitors with AC Line Filtering Performance. Angewandte Chemie - International Edition, 2017, 56, 3920-3924.	7.2	140
13	Engineering crystalline quasi-two-dimensional polyaniline thin film with enhanced electrical and chemiresistive sensing performances. Nature Communications, 2019, 10, 4225.	5.8	132
14	Reusability of photocatalytic TiO <sub>2</sub> and ZnO nanoparticles immobilized in poly(vinylidene fluoride) overlayers. Nature Communications, 2019, 10, 222.	8.1	122
15	Synthesis of NBN-Type Zigzag-Edged Polycyclic Aromatic Hydrocarbons: 1,9-Diaza-9a-boraphenalene as a Structural Motif. Journal of the American Chemical Society, 2016, 138, 11606-11615.	6.6	121
16	Resonant Electron Heating and Molecular Phonon Cooling in Single-Carbon Nanotube Junctions. Physical Review Letters, 2008, 100, 136801.	2.9	120
17	Vibrational modes and low-temperature thermal properties of graphene and carbon nanotubes: Minimal force-constant model. Physical Review B, 2008, 78, .	1.1	117
18	A bottom-up route to enhance thermoelectric figures of merit in graphene nanoribbons. Scientific Reports, 2013, 3, 1228.	1.6	117

#	ARTICLE	IF	CITATIONS
19	Two-Dimensional Boronate Ester Covalent Organic Framework Thin Films with Large Single Crystalline Domains for a Neuromorphic Memory Device. <i>Angewandte Chemie - International Edition</i> , 2020, 59, 8218-8224.	7.2	116
20	Non-equilibrium Green's functions in density functional tight binding: method and applications. <i>New Journal of Physics</i> , 2008, 10, 065022.	1.2	111
21	Incoherent Electron-Phonon Scattering in Octanethiols. <i>Nano Letters</i> , 2004, 4, 2109-2114.	4.5	106
22	Understanding the inelastic electron-tunneling spectra of alkanedithiols on gold. <i>Journal of Chemical Physics</i> , 2006, 124, 094704.	1.2	103
23	Insight into doping efficiency of organic semiconductors from the analysis of the density of states in n-doped C60 and ZnPc. <i>Nature Materials</i> , 2018, 17, 439-444.	13.3	101
24	Impact of molecular quadrupole moments on the energy levels at organic heterojunctions. <i>Nature Communications</i> , 2019, 10, 2466.	5.8	101
25	Multimetallic Hierarchical Aerogels: Shape Engineering of the Building Blocks for Efficient Electrocatalysis. <i>Advanced Materials</i> , 2017, 29, 1605254.	11.1	98
26	The Multiscale Paradigm in Electronic Device Simulation. <i>IEEE Transactions on Electron Devices</i> , 2011, 58, 1425-1432.	1.6	97
27	Dodecacene Generated on Surface: Reopening of the Energy Gap. <i>ACS Nano</i> , 2020, 14, 1011-1017.	7.3	93
28	Mechanical properties of polycrystalline boron-nitride nanosheets. <i>RSC Advances</i> , 2014, 4, 19137-19143.	1.7	90
29	A Stable Saddle-Shaped Polycyclic Hydrocarbon with an Open-Shell Singlet Ground State. <i>Angewandte Chemie - International Edition</i> , 2017, 56, 3280-3284.	7.2	90
30	Persulfurated Coronene: A New Generation of "Sulflower". <i>Journal of the American Chemical Society</i> , 2017, 139, 2168-2171.	6.6	89
31	Theory of heat dissipation in molecular electronics. <i>Physical Review B</i> , 2007, 75, .	1.1	88
32	Effects of Al-doping on the properties of Li-Mn-Ni-O cathode materials for Li-ion batteries: an ab initio study. <i>Journal of Materials Chemistry A</i> , 2013, 1, 9273.	5.2	84
33	Anisotropic Thermoelectric Response in Two-Dimensional Puckered Structures. <i>Journal of Physical Chemistry C</i> , 2016, 120, 18841-18849.	1.5	84
34	Understanding the catalyst-free transformation of amorphous carbon into graphene by current-induced annealing. <i>Scientific Reports</i> , 2013, 3, .	1.6	82
35	A priorimethod for propensity rules for inelastic electron tunneling spectroscopy of single-molecule conduction. <i>Physical Review B</i> , 2007, 75, .	1.1	80
36	Combined density functional theory and Landauer approach for hole transfer in DNA along classical molecular dynamics trajectories. <i>Journal of Chemical Physics</i> , 2009, 130, 215104.	1.2	78

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37	High-Performance Three-Dimensional Tubular Nanomembrane Sensor for DNA Detection. Nano Letters, 2016, 16, 4288-4296.	4.5	78
38	Role of Ferroelectric Nanodomains in the Transport Properties of Perovskite Solar Cells. Nano Letters, 2016, 16, 988-992.	4.5	75
39	A Chirality-Based Quantum Leap. ACS Nano, 2022, 16, 4989-5035.	7.3	74
40	Tailorable Acceptor-C60 and Donor-C60 Molecules Pairs for Molecular Electronics. Physical Review Letters, 2003, 90, 206602.	2.9	73
41	Modeling extended contacts for nanotube and graphene devices. Physical Review B, 2008, 77, .	1.1	71
42	Theoretical Insight into High-Efficiency Triple-Junction Tandem Solar Cells via the Band Engineering of Antimony Chalcogenides. Solar Rrl, 2021, 5, 2000800.	3.1	70
43	Negative Photoconductance in Heavily Doped Si Nanowire Field-Effect Transistors. Nano Letters, 2017, 17, 6727-6734.	4.5	69
44	Enhanced Magnetoresistance in Chiral Molecular Junctions. Journal of Physical Chemistry Letters, 2018, 9, 5453-5459.	2.1	69
45	Electrochemically Exfoliated High-Quality 2H-MoS <sub>2</sub> for Multiflake Thin Film Flexible Biosensors. Small, 2019, 15, e1901265.	5.2	65
46	Exciton Binding Energy in Molecular Triads. Journal of Physical Chemistry C, 2017, 121, 17088-17095.	1.5	64
47	Silicon nanowires – a versatile technology platform. Physica Status Solidi - Rapid Research Letters, 2013, 7, 793-799.	1.2	61
48	Applications of 2D-Layered Palladium Diselenide and Its van der Waals Heterostructures in Electronics and Optoelectronics. Nano-Micro Letters, 2021, 13, 143.	14.4	61
49	Tetracene Formation by On-Surface Reduction. ACS Nano, 2016, 10, 4538-4542.	7.3	60
50	Few-Layer Graphene Kills Selectively Tumor Cells from Myelomonocytic Leukemia Patients. Angewandte Chemie - International Edition, 2017, 56, 3014-3019.	7.2	59
51	Enhancing single-parameter quantum charge pumping in carbon-based devices. Applied Physics Letters, 2011, 99, 092102.	1.5	58
52	Light Weight and Flexible High-Performance Diagnostic Platform. Advanced Healthcare Materials, 2015, 4, 1517-1525.	3.9	58
53	Nonlinear Work Function Tuning of Lead-Halide Perovskites by MXenes with Mixed Terminations. Advanced Functional Materials, 2020, 30, 1909028.	7.8	58
54	Spin-valve effect in zigzag graphene nanoribbons by defect engineering. Physical Review B, 2009, 80, .	1.1	56

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55	A Dual-Stimuli-Responsive Sodium-Bromine Battery with Ultrahigh Energy Density. <i>Advanced Materials</i> , 2018, 30, e1800028.	11.1	56
56	High-Motility Visible Light-Driven Ag/AgCl Janus Micromotors. <i>Small</i> , 2018, 14, e1803613.	5.2	56
57	Parallel arrays of Schottky barrier nanowire field effect transistors: Nanoscopic effects for macroscopic current output. <i>Nano Research</i> , 2013, 6, 381-388.	5.8	55
58	Decacene: On-Surface Generation. <i>Angewandte Chemie</i> , 2017, 129, 12107-12110.	1.6	54
59	Controlling the conductance and noise of driven carbon-based Fabry-Pérot devices. <i>Applied Physics Letters</i> , 2009, 94, .	1.5	52
60	On the importance of ferroelectric domains for the performance of perovskite solar cells. <i>Nano Energy</i> , 2018, 48, 20-26.	8.2	52
61	Straintronics in graphene: Extra large electronic band gap induced by tensile and shear strains. <i>Journal of Applied Physics</i> , 2019, 126, .	1.1	51
62	Enhanced Photocatalytic Activity of Au/TiO <sub>2</sub> Nanoparticles against Ciprofloxacin. <i>Catalysts</i> , 2020, 10, 234.	1.6	50
63	Disorder and dephasing effects on electron transport through conjugated molecular wires in molecular junctions. <i>Physical Review B</i> , 2012, 85, .	1.1	48
64	Materials Meets Concepts in Molecule-Based Electronics. <i>Advanced Functional Materials</i> , 2015, 25, 1933-1954.	7.8	47
65	Charge-carrier mobilities in binary mixtures of discotic triphenylene derivatives as a function of temperature. <i>Physical Review B</i> , 2002, 65, .	1.1	46
66	Efficient linear scaling method for computing the thermal conductivity of disordered materials. <i>Physical Review B</i> , 2011, 83, .	1.1	46
67	Synthesis of Wafer-Scale Graphene with Chemical Vapor Deposition for Electronic Device Applications. <i>Advanced Materials Technologies</i> , 2021, 6, 2000744.	3.0	46
68	Nucleobase adsorbed at graphene devices: Enhance bio-sensorics. <i>Applied Physics Letters</i> , 2012, 100, 063101.	1.5	45
69	Schottky barrier-based silicon nanowire pH sensor with live sensitivity control. <i>Nano Research</i> , 2014, 7, 263-271.	5.8	45
70	Graphene Biodevices for Early Disease Diagnosis Based on Biomarker Detection. <i>ACS Sensors</i> , 2021, 6, 3841-3881.	4.0	45
71	Applications of nanogenerators for biomedical engineering and healthcare systems. <i>Informa Materials</i> , 2022, 4, .	8.5	45
72	Chirality-Induced Spin Selectivity in a Coarse-Grained Tight-Binding Model for Helicene. <i>Journal of Physical Chemistry C</i> , 2019, 123, 27230-27241.	1.5	44

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73	Schottky barrier height at an organic/metal junction: A first-principles study of PTCDA/X(X=Al,Ag)contacts. <i>Physical Review B</i> , 2003, 68, .	1.1	43
74	Ultrasensitive detection of Ebola matrix protein in a memristor mode. <i>Nano Research</i> , 2018, 11, 1057-1068.	5.8	43
75	Molecular Origins of Conduction Channels Observed in Shot-Noise Measurements. <i>Nano Letters</i> , 2006, 6, 2431-2437.	4.5	42
76	Electronic Resonances and Gap Stabilization of Higher Acenes on a Gold Surface. <i>ACS Nano</i> , 2018, 12, 8506-8511.	7.3	42
77	Phonon transport in large scale carbon-based disordered materials: Implementation of an efficient order- $\langle \text{mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline">\langle \text{mml:mi} \rangle N \langle \text{mml:math} \rangle$ and real-space Kubo methodology. <i>Physical Review B</i> , 2010, 82, .	1.1	41
78	Fully $sp^2$ -Carbon-Linked Crystalline Two-Dimensional Conjugated Polymers: Insight into 2D Poly(phenylenecyanovinylene) Formation and its Optoelectronic Properties. <i>Chemistry - A European Journal</i> , 2019, 25, 6562-6568.	1.7	40
79	Photoconductive transients and one-dimensional charge carrier dynamics in discotic liquid crystals. <i>Physical Review B</i> , 2002, 65, .	1.1	38
80	Vibrational effects in the linear conductance of carbon nanotubes. <i>Europhysics Letters</i> , 2005, 71, 438-444.	0.7	38
81	Molecular junctions in the Coulomb blockade regime: Rectification and nesting. <i>Physical Review B</i> , 2007, 76, .	1.1	38
82	Heating and cooling mechanisms in single-molecule junctions. <i>Physical Review B</i> , 2010, 81, .	1.1	37
83	Compact Nanowire Sensors Probe Microdroplets. <i>Nano Letters</i> , 2016, 16, 4991-5000.	4.5	37
84	Electrochemical detection of ascorbic acid in artificial sweat using a flexible alginate/CuO-modified electrode. <i>Mikrochimica Acta</i> , 2020, 187, 520.	2.5	37
85	Intrinsic plasticity of silicon nanowire neurotransistors for dynamic memory and learning functions. <i>Nature Electronics</i> , 2020, 3, 398-408.	13.1	37
86	Strong Overtones Modes in Inelastic Electron Tunneling Spectroscopy with Cross-Conjugated Molecules: A Prediction from Theory. <i>ACS Nano</i> , 2013, 7, 9183-9194.	7.3	36
87	Influence of side groups on the performance of infrared absorbing aza-BODIPY organic solar cells. <i>Physica Status Solidi (A) Applications and Materials Science</i> , 2015, 212, 2747-2753.	0.8	35
88	Role of Exchange Interactions in the Magnetic Response and Intermolecular Recognition of Chiral Molecules. <i>Nano Letters</i> , 2020, 20, 7077-7086.	4.5	35
89	Combined effect of strain and defects on the conductance of graphene nanoribbons. <i>Physical Review B</i> , 2013, 88, .	1.1	34
90	Confined Catalytic Janus Swimmers in a Crowded Channel: Geometry-Driven Rectification Transients and Directional Locking. <i>Small</i> , 2016, 12, 5882-5890.	5.2	34

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91	On-water surface synthesis of charged two-dimensional polymer single crystals via the irreversible Katritzky reaction. , 2022, 1, 69-76.		34
92	The symmetry of single-molecule conduction. Journal of Chemical Physics, 2006, 125, 184702.	1.2	33
93	The Green's Function Density Functional Tight-Binding (gDFTB) Method for Molecular Electronic Conduction. Journal of Physical Chemistry A, 2007, 111, 5692-5702.	1.1	32
94	Electronic and transport properties of silicon nanowires. Journal of Computational Electronics, 2007, 6, 329-333.	1.3	32
95	Silicon-based molecular switch junctions. Nano Research, 2009, 2, 648-659.	5.8	32
96	Optoelectronic switching of nanowire-based hybrid organic/oxide/semiconductor field-effect transistors. Nano Research, 2015, 8, 1229-1240.	5.8	32
97	Stimulation of bone formation by monocyte-activator functionalized graphene oxide <i>in vivo</i>. Nanoscale, 2019, 11, 19408-19421.	2.8	32
98	Two-Dimensional SiP, SiAs, GeP and GeAs as Promising Candidates for Photocatalytic Applications. Coatings, 2019, 9, 522.	1.2	32
99	Photocatalytic Microporous Membrane against the Increasing Problem of Water Emerging Pollutants. Materials, 2019, 12, 1649.	1.3	32
100	High-performance electronics and optoelectronics of monolayer tungsten diselenide full film from pre-seeding strategy. Informa Mater, 2021, 3, 1455-1469.	8.5	32
101	Scaling and Graphical Transport-Map Analysis of Ambipolar Schottky-Barrier Thin-Film Transistors Based on a Parallel Array of Si Nanowires. Nano Letters, 2015, 15, 4578-4584.	4.5	31
102	Tuning Near-Infrared Absorbing Donor Materials: A Study of Electronic, Optical, and Charge-Transport Properties of aza-BODIPYs. Chemistry of Materials, 2017, 29, 5525-5536.	3.2	31
103	Determining the Diffusion Coefficient of Lithium Insertion Cathodes from GITT measurements: Theoretical Analysis for low Temperatures**. ChemPhysChem, 2021, 22, 885-893.	1.0	30
104	Negative quantum capacitance of gated carbon nanotubes. Physical Review B, 2005, 72, .	1.1	29
105	Unveiling the Atomic Structure of Single-Wall Boron Nanotubes. Advanced Functional Materials, 2014, 24, 4127-4134.	7.8	29
106	Thermal bridging of graphene nanosheets via covalent molecular junctions: A non-equilibrium Green's functions density functional tight-binding study. Nano Research, 2019, 12, 791-799.	5.8	29
107	Role of thermal vibrations in molecular wire conduction. Physical Review B, 2003, 68, .	1.1	28
108	Permittivity of Oxidized Ultra-Thin Silicon Films From Atomistic Simulations. IEEE Electron Device Letters, 2015, 36, 1076-1078.	2.2	28

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109	Thermal Decoherence and Disorder Effects on Chiral-Induced Spin Selectivity. <i>Journal of Physical Chemistry Letters</i> , 2018, 9, 5753-5758.	2.1	28
110	Applications of Carbon Nanotubes in the Internet of Things Era. <i>Nano-Micro Letters</i> , 2021, 13, 191.	14.4	28
111	Light-field characterization in a continuous hydrogen-producing photobioreactor by optical simulation and computational fluid dynamics. <i>Biotechnology and Bioengineering</i> , 2015, 112, 2439-2449.	1.7	27
112	SCC-DFTB Parametrization for Boron and Boranes. <i>Journal of Chemical Theory and Computation</i> , 2012, 8, 1153-1163.	2.3	26
113	Modeling charge transport in DNA using multi-scale methods. <i>Physica Status Solidi (B): Basic Research</i> , 2013, 250, 2277-2287.	0.7	26
114	Switchable Negative Differential Resistance Induced by Quantum Interference Effects in Porphyrin-based Molecular Junctions. <i>Journal of Physical Chemistry Letters</i> , 2015, 6, 3950-3955.	2.1	26
115	From Fluorine to Fluorene—A Route to Thermally Stable azabodipyrene (BODIPYs) for Organic Solar Cell Application. <i>Advanced Electronic Materials</i> , 2016, 2, 1600152.	2.6	26
116	In-Situ Stretching Patterned Graphene Nanoribbons in the Transmission Electron Microscope. <i>Scientific Reports</i> , 2017, 7, 211.	1.6	26
117	Nanosensor-Based Real-Time Monitoring of Stress Biomarkers in Human Saliva Using a Portable Measurement System. <i>ACS Sensors</i> , 2020, 5, 4081-4091.	4.0	26
118	Enhanced visible-light photodegradation of fluoroquinolone-based antibiotics and <i>E. coli</i> growth inhibition using Ag <sub>2</sub> TiO <sub>2</sub> nanoparticles. <i>RSC Advances</i> , 2021, 11, 13980-13991.	1.7	26
119	Ultrahigh Electron Thermal Conductivity in Graphene, Biphenylene, and Net Graphene. <i>Advanced Energy Materials</i> , 2022, 12, .	10.2	26
120	TiberCAD: towards multiscale simulation of optoelectronic devices. <i>Optical and Quantum Electronics</i> , 2008, 40, 1077-1083.	1.5	25
121	A parabolic model to control quantum interference in T-shaped molecular junctions. <i>Physical Chemistry Chemical Physics</i> , 2013, 15, 13951.	1.3	25
122	Model of a realistic InP surface quantum dot extrapolated from atomic force microscopy results. <i>Nanotechnology</i> , 2014, 25, 195201.	1.3	25
123	Boron-Doped Single-Walled Carbon Nanotubes with Enhanced Thermoelectric Power Factor for Flexible Thermoelectric Devices. <i>ACS Applied Energy Materials</i> , 2020, 3, 2556-2564.	2.5	25
124	Electron-phonon scattering in molecular electronics: from inelastic electron tunnelling spectroscopy to heating effects. <i>New Journal of Physics</i> , 2008, 10, 065020.	1.2	24
125	Unimolecular Logic Gate with Classical Input by Single Gold Atoms. <i>ACS Nano</i> , 2018, 12, 1139-1145.	7.3	24
126	Effective Hamiltonian model for helically constrained quantum systems within adiabatic perturbation theory: Application to the chirality-induced spin selectivity (CISS) effect. <i>Journal of Chemical Physics</i> , 2020, 152, 214105.	1.2	24



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127	Polycyclic heteroaromatic hydrocarbons containing a benzoisindole core. <i>Organic Chemistry Frontiers</i> , 2017, 4, 847-852.	2.3	23
128	Edge magnetism impact on electrical conductance and thermoelectric properties of graphenelike nanoribbons. <i>Physical Review B</i> , 2017, 96, .	1.1	23
129	Emerging Internet of Things driven carbon nanotubes-based devices. <i>Nano Research</i> , 2022, 15, 4613-4637.	5.8	23
130	Coordination Polymer Framework Based On a Chip Micro-Supercapacitors with AC Line Filtering Performance. <i>Angewandte Chemie</i> , 2017, 129, 3978-3982.	1.6	22
131	Bottom-up synthesis of ultrathin straight platinum nanowires: Electric field impact. <i>Nano Research</i> , 2013, 6, 303-311.	5.8	21
132	Enhanced thermoelectric figure of merit in polycrystalline carbon nanostructures. <i>Physical Review B</i> , 2015, 92, .	1.1	21
133	Bipolar nitrogen-doped graphene frameworks as high-performance cathodes for lithium ion batteries. <i>Journal of Materials Chemistry A</i> , 2017, 5, 1588-1594.	5.2	21
134	Density Functional Tight Binding for Quantum Plasmonics. <i>Journal of Physical Chemistry C</i> , 2018, 122, 19756-19766.	1.5	21
135	Simulating random alloy effects in III-nitride light emitting diodes. <i>Journal of Applied Physics</i> , 2020, 128, 041102.	1.1	21
136	Selective and self-validating breath-level detection of hydrogen sulfide in humid air by gold nanoparticle-functionalized nanotube arrays. <i>Nano Research</i> , 2022, 15, 2512-2521.	5.8	21
137	IETS and quantum interference: Propensity rules in the presence of an interference feature. <i>Journal of Chemical Physics</i> , 2014, 141, 124119.	1.2	20
138	Copper Induced Conformational Changes of Tripeptide Monolayer Based Impedimetric Biosensor. <i>Scientific Reports</i> , 2017, 7, 9498.	1.6	20
139	Polymerization driven monomer passage through monolayer chemical vapour deposition graphene. <i>Nature Communications</i> , 2018, 9, 4051.	5.8	20
140	Boron Doping of SWCNTs as a Way to Enhance the Thermoelectric Properties of Melt-Mixed Polypropylene/SWCNT Composites. <i>Energies</i> , 2020, 13, 394.	1.6	20
141	The Role of Contacts in Molecular Electronics. , 2002, , 133-149.		20
142	Tuning quantum electron and phonon transport in two-dimensional materials by strain engineering: a Green's function based study. <i>Physical Chemistry Chemical Physics</i> , 2017, 19, 1487-1495.	1.3	19
143	Inverse Solidification Induced by Active Janus Particles. <i>Advanced Functional Materials</i> , 2020, 30, 2003851.	7.8	19
144	Coupling of molecular vibrons with contact phonon reservoirs. <i>Journal of Physics Condensed Matter</i> , 2007, 19, 215207.	0.7	18

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145	Quantum transport through STM-lifted single PTCDA molecules. Applied Physics A: Materials Science and Processing, 2008, 93, 335-343.	1.1	18
146	Light-Induced Contraction/Expansion of 1D Photoswitchable Metallopolymer Monitored at the Solid-Liquid Interface. Small, 2017, 13, 1701790.	5.2	18
147	On-Surface Annulation Reaction Cascade for the Selective Synthesis of Diindenopyrene. ACS Nano, 2017, 11, 12419-12425.	7.3	18
148	Gating Hysteresis as an Indicator for Silicon Nanowire FET Biosensors. Applied Sciences (Switzerland), 2018, 8, 950.	1.3	18
149	Surface Modification of Silicon Nanowire Based Field Effect Transistors with Stimuli Responsive Polymer Brushes for Biosensing Applications. Micromachines, 2020, 11, 274.	1.4	18
150	Machine Learning-Enabled Smart Gas Sensing Platform for Identification of Industrial Gases. Advanced Intelligent Systems, 2022, 4, .	3.3	18
151	Atomistic Modeling of Charge Transport across a Carbon Nanotube-Polyethylene Junction. Journal of Physical Chemistry C, 2013, 117, 8020-8027.	1.5	17
152	Developing a Customized Perfusion Bioreactor Prototype with Controlled Positional Variability in Oxygen Partial Pressure for Bone and Cartilage Tissue Engineering. Tissue Engineering - Part C: Methods, 2017, 23, 286-297.	1.1	17
153	First-Principle-Based Phonon Transport Properties of Nanoscale Graphene Grain Boundaries. Advanced Science, 2018, 5, 1700365.	5.6	17
154	Anisotropic Exclusion Effect between Photocatalytic Ag/AgCl Janus Particles and Passive Beads in a Dense Colloidal Matrix. Langmuir, 2020, 36, 7091-7099.	1.6	17
155	Atomistic Modeling of Gate-All-Around Si-Nanowire Field-Effect Transistors. IEEE Transactions on Electron Devices, 2007, 54, 3159-3167.	1.6	16
156	Enhanced $\pi$ - $\pi$ interactions between a C60 fullerene and a buckle bend on a double-walled carbon nanotube. Nano Research, 2010, 3, 92-97.	5.8	16
157	Model of a GaAs Quantum Dot Embedded in a Polymorph AlGaAs Nanowire. IEEE Journal of Selected Topics in Quantum Electronics, 2013, 19, 1-9.	1.9	16
158	Electron transport in extended carbon-nanotube/metal contacts: <i>Ab initio</i> based Green function method. Physical Review B, 2015, 91, .	1.1	16
159	Monitoring microbial metabolites using an inductively coupled resonance circuit. Scientific Reports, 2015, 5, 12878.	1.6	16
160	Scaling of the conductance in gold nanotubes. Physical Review B, 2006, 74, .	1.1	15
161	Atomistic simulations of InGaN/GaN random alloy quantum well LEDs. Physica Status Solidi C: Current Topics in Solid State Physics, 2014, 11, 632-634.	0.8	15
162	Dynamic Effects on the Charge Transport in an Organic Near-Infrared Absorber Material. Journal of Physical Chemistry C, 2014, 118, 6537-6547.	1.5	15

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163	DFT study of interaction of additives with Cu(111) surface relevant to Cu electrodeposition. Journal of Applied Electrochemistry, 2018, 48, 211-219.	1.5	15
164	Introducing Molecular Electronics: A Brief Overview. , 2006, , 1-10.		14
165	DFT Modeling of Bulk-Modulated Carbon Nanotube Field-Effect Transistors. IEEE Nanotechnology Magazine, 2007, 6, 13-21.	1.1	14
166	Charge Migration in Organic Materials: Can Propagating Charges Affect the Key Physical Quantities Controlling Their Motion?. Israel Journal of Chemistry, 2012, 52, 452-460.	1.0	14
167	Coupling atomistic and continuous media models for electronic device simulation. Journal of Computational Electronics, 2013, 12, 553-562.	1.3	14
168	Influence of electromechanical coupling on optical properties of InGaN quantum-dot based light-emitting diodes. Nanotechnology, 2017, 28, 015701.	1.3	14
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