

Wolfgang Wenzel

List of Publications by Year in Descending Order

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The third column is the impact factor (IF) of the journal, and the fourth column is the number of citations of the article.

269
papers

7,104
citations

45
h-index

67
g-index

299
ext. papers

8,062
ext. citations

6.6
avg, IF

6.1
L-index

#	Paper	IF	Citations
269	Impact of the Polymorphism and Relativistic Effects on the Electronic Properties of Inorganic Metal Halide Perovskites. <i>Journal of Physical Chemistry C</i> , 2022 , 126, 2131-2140	3.8	1
268	Simulating the growth of amorphous organic thin films. <i>Organic Electronics</i> , 2022 , 102, 106439	3.5	0
267	Modelling peptide adsorption energies on gold surfaces with an effective implicit solvent and surface model. <i>Journal of Colloid and Interface Science</i> , 2022 , 605, 493-499	9.3	0
266	Photostationary State in Dynamic Covalent Networks.. <i>ACS Macro Letters</i> , 2022 , 11, 532-536	6.6	0
265	Challenges and limits of mechanical stability in 3D direct laser writing.. <i>Nature Communications</i> , 2022 , 13, 2115	17.4	5
264	Editorial to the Special Issue: How to Reinvent the Ways to Invent the Batteries of the Future [The Battery 2030+ Large-Scale Research Initiative Roadmap. <i>Advanced Energy Materials</i> , 2022 , 12, 2200644	21.8	0
263	Systematic kMC Study of Doped Hole Injection Layers in Organic Electronics.. <i>Frontiers in Chemistry</i> , 2021 , 9, 809415	5	1
262	De Novo Calculation of the Charge Carrier Mobility in Amorphous Small Molecule Organic Semiconductors.. <i>Frontiers in Chemistry</i> , 2021 , 9, 801589	5	2
261	Tough, Transparent, 3D printable and Self-healing Polyethylene Glycol-Gel (PEGgel). <i>Advanced Materials</i> , 2021 , e2107791	24	7
260	Action Plots in Action: In-Depth Insights into Photochemical Reactivity. <i>Journal of the American Chemical Society</i> , 2021 ,	16.4	9
259	Fast Generation of Machine Learning-Based Force Fields for Adsorption Energies. <i>Journal of Chemical Theory and Computation</i> , 2021 , 17, 7195-7202	6.4	1
258	Monte-Carlo Simulations of Soft Matter Using SIMONA: A Review of Recent Applications. <i>Frontiers in Physics</i> , 2021 , 9,	3.9	1
257	Structural and Dynamic Insights into the Conduction of Lithium-Ionic-Liquid Mixtures in Nanoporous Metal-Organic Frameworks as Solid-State Electrolytes. <i>ACS Applied Materials & Interfaces</i> , 2021 , 13, 21166-21174	9.5	6
256	Adsorption of organic molecules on carbon surfaces: Experimental data and molecular dynamics simulation considering multiple protonation states. <i>Journal of Colloid and Interface Science</i> , 2021 , 589, 424-437	9.3	9
255	22-3: Tuning ETL Mobility by Disorder Passivation. <i>Digest of Technical Papers SID International Symposium</i> , 2021 , 52, 270-273	0.5	
254	Analyzing Dynamical Disorder for Charge Transport in Organic Semiconductors via Machine Learning. <i>Journal of Chemical Theory and Computation</i> , 2021 , 17, 3750-3759	6.4	5
253	Computing Charging and Polarization Energies of Small Organic Molecules Embedded into Amorphous Materials with Quantum Accuracy. <i>Journal of Chemical Theory and Computation</i> , 2021 , 17, 3727-3738	6.4	2

252	DNA Binding to the Silica: Cooperative Adsorption in Action. <i>Langmuir</i> , 2021 , 37, 5902-5908	4	5
251	Encapsulation of Au ₅₅ Clusters within Surface-Supported Metal-Organic Frameworks for Catalytic Reduction of 4-Nitrophenol. <i>ACS Applied Nano Materials</i> , 2021 , 4, 522-528	5.6	5
250	Modular functionalization and hydrogel formation red-shifted and self-reporting [2+2] cycloadditions. <i>Chemical Communications</i> , 2021 , 57, 805-808	5.8	8
249	A coarse-grained xDLVO model for colloidal protein-protein interactions. <i>Physical Chemistry Chemical Physics</i> , 2021 , 23, 12780-12794	3.6	4
248	Structural design of pyrene-functionalized TEMPO-containing polymers for enhanced electrochemical storage performance. <i>Polymer Chemistry</i> , 2021 , 12, 2643-2650	4.9	3
247	Green light LED activated ligation of a scalable, versatile chalcone chromophore. <i>Polymer Chemistry</i> , 2021 , 12, 4903-4909	4.9	5
246	Interplay of structural dynamics and electronic effects in an engineered assembly of pentacene in a metal-organic framework. <i>Chemical Science</i> , 2021 , 12, 4477-4483	9.4	6
245	Enantiomeric Separation of Semiconducting Single-Walled Carbon Nanotubes by Acid Cleavable Chiral Polyfluorene. <i>ACS Nano</i> , 2021 , 15, 4699-4709	16.7	9
244	Ionic liquid gating of single-walled carbon nanotube devices with ultra-short channel length down to 10 nm. <i>Applied Physics Letters</i> , 2021 , 118, 063101	3.4	2
243	Avoiding the Center-Symmetry Trap: Programmed Assembly of Dipolar Precursors into Porous, Crystalline Molecular Thin Films. <i>Advanced Materials</i> , 2021 , 33, e2103287	24	1
242	Wavelength-Selective Softening of Hydrogel Networks. <i>Advanced Materials</i> , 2021 , 33, e2102184	24	10
241	Fluorescent Nanozeolite Receptors for the Highly Selective and Sensitive Detection of Neurotransmitters in Water and Biofluids. <i>Advanced Materials</i> , 2021 , e2104614	24	2
240	Insights on Alanine and Arginine Binding to Silica with Atomic Resolution. <i>Journal of Physical Chemistry Letters</i> , 2021 , 12, 9384-9390	6.4	1
239	De Novo Simulation of Charge Transport through Organic Single-Carrier Devices. <i>Journal of Chemical Theory and Computation</i> , 2021 , 17, 6416-6422	6.4	2
238	Optical and Electrical Measurements Reveal the Orientation Mechanism of Homoleptic Iridium-Carbene Complexes. <i>ACS Applied Materials & Interfaces</i> , 2020 , 12, 51709-51718	9.5	4
237	Conductive Metal-Organic Framework Thin Film Hybrids by Electropolymerization of Monosubstituted Acetylenes. <i>ACS Applied Materials & Interfaces</i> , 2020 , 12, 30972-30979	9.5	8
236	Macromolecular Superstructures: A Future Beyond Single Chain Nanoparticles. <i>Israel Journal of Chemistry</i> , 2020 , 60, 86-99	3.4	33
235	Stability of hexafluoroacetylacetone molecules on metallic and oxidized nickel surfaces in atomic-layer-etching processes. <i>Journal of Vacuum Science and Technology A: Vacuum, Surfaces and Films</i> , 2020 , 38, 022610	2.9	6

234	Wavelength-gated photoreversible polymerization and topology control. <i>Chemical Science</i> , 2020 , 11, 2834-2842	9.4	15
233	Wavelength-Dependent Stiffening of Hydrogel Matrices via Redshifted [2+2] Photocycloadditions. <i>Advanced Functional Materials</i> , 2020 , 30, 1908171	15.6	31
232	Multiscale Simulation of Photoluminescence Quenching in Phosphorescent OLED Materials. <i>Advanced Theory and Simulations</i> , 2020 , 3, 1900222	3.5	10
231	Disorder-driven doping activation in organic semiconductors. <i>Physical Chemistry Chemical Physics</i> , 2020 , 22, 10256-10264	3.6	10
230	43-3: Ab-initio Simulation of Doped Injection Layers.. <i>Digest of Technical Papers SID International Symposium</i> , 2020 , 51, 630-633	0.5	6
229	Photocycloadditions in disparate chemical environments. <i>Chemical Communications</i> , 2020 , 56, 14043-14045	3.4	8
228	Photocycloreversions within single polymer chains. <i>Polymer Chemistry</i> , 2020 , 11, 6616-6623	4.9	4
227	Multi-material 3D microstructures with photochemically adaptive mechanical properties. <i>Journal of Materials Chemistry C</i> , 2020 , 8, 10993-11000	7.1	6
226	Formation and desorption of nickel hexafluoroacetylacetonate Ni(hfac) ₂ on a nickel oxide surface in atomic layer etching processes. <i>Journal of Vacuum Science and Technology A: Vacuum, Surfaces and Films</i> , 2020 , 38, 052602	2.9	7
225	Sampling of the conformational landscape of small proteins with Monte Carlo methods. <i>Scientific Reports</i> , 2020 , 10, 18211	4.9	7
224	Green light triggered [2+2] cycloaddition of halochromic styrylquinoxaline-controlling photoreactivity by pH. <i>Nature Communications</i> , 2020 , 11, 4193	17.4	22
223	Tuning Optical Properties by Controlled Aggregation: Electroluminescence Assisted by Thermally-Activated Delayed Fluorescence from Thin Films of Crystalline Chromophores. <i>Chemistry - A European Journal</i> , 2020 , 26, 17016-17020	4.8	18
222	Buffer Influence on the Amino Acid Silica Interaction. <i>ChemPhysChem</i> , 2020 , 21, 2347-2356	3.2	7
221	Tacticity dependence of single chain polymer folding. <i>Polymer Chemistry</i> , 2020 , 11, 3439-3445	4.9	3
220	Method for accurate experimental determination of singlet and triplet exciton diffusion between thermally activated delayed fluorescence molecules. <i>Chemical Science</i> , 2020 , 12, 1121-1125	9.4	5
219	Light-fueled dynamic covalent crosslinking of single polymer chains in non-equilibrium states. <i>Chemical Science</i> , 2020 , 12, 1302-1310	9.4	6
218	Concentration dependent energy levels shifts in donor-acceptor mixtures due to intermolecular electrostatic interaction. <i>Scientific Reports</i> , 2019 , 9, 12424	4.9	5
217	Rational Design of Iron Oxide Binding Peptide Tags. <i>Langmuir</i> , 2019 , 35, 8472-8481	4	4

216	19-4: Boosting OLED Performance with Ab-initio Modeling of Roll-off and Quenching Processes. <i>Digest of Technical Papers SID International Symposium, 2019, 50, 259-262</i>	0.5	6
215	Tailoring the Mechanical Properties of 3D Microstructures Using Visible Light Post-Manufacturing. <i>Advanced Materials, 2019, 31, e1901269</i>	24	27
214	Triplet exciton diffusion in metalorganic phosphorescent host-guest systems from first principles. <i>Physical Review B, 2019, 99,</i>	3.3	12
213	Toward Design of Novel Materials for Organic Electronics. <i>Advanced Materials, 2019, 31, e1808256</i>	24	60
212	A de novo strategy for predictive crystal engineering to tune excitonic coupling. <i>Nature Communications, 2019, 10, 2048</i>	17.4	27
211	Photoleitfähigkeit in Dünfilmen Metall-organischer Gerüste. <i>Angewandte Chemie, 2019, 131, 9691-9696</i>	3.6	12
210	Photoconductivity in Metal-Organic Framework (MOF) Thin Films. <i>Angewandte Chemie - International Edition, 2019, 58, 9590-9595</i>	16.4	68
209	Bunching and Immobilization of Ionic Liquids in Nanoporous Metal-Organic Framework. <i>Nano Letters, 2019, 19, 2114-2120</i>	11.5	31
208	Disorder compensation controls doping efficiency in organic semiconductors. <i>Nature Communications, 2019, 10, 4547</i>	17.4	23
207	Light-Switchable One-Dimensional Photonic Crystals Based on MOFs with Photomodulatable Refractive Index. <i>Journal of Physical Chemistry Letters, 2019, 10, 6626-6633</i>	6.4	11
206	Host dependence of the electron affinity of molecular dopants. <i>Materials Horizons, 2019, 6, 107-114</i>	14.4	44
205	Contemporary Photoligation Chemistry: The Visible Light Challenge. <i>Chemistry - A European Journal, 2019, 25, 3700-3709</i>	4.8	23
204	Lichtinduziertes Schalten der Leitfähigkeit von MOFs mit eingelagertem Spiropyran. <i>Angewandte Chemie, 2019, 131, 1205-1210</i>	3.6	18
203	Controlling Chain Coupling and Single-Chain Ligation by Two Colours of Visible Light. <i>Angewandte Chemie - International Edition, 2019, 58, 3604-3609</i>	16.4	43
202	Conductance Photoswitching of Metal-Organic Frameworks with Embedded Spiropyran. <i>Angewandte Chemie - International Edition, 2019, 58, 1193-1197</i>	16.4	74
201	Access to Disparate Soft Matter Materials by Curing with Two Colors of Light. <i>Advanced Materials, 2019, 31, e1807288</i>	24	43
200	Full quantum treatment of charge dynamics in amorphous molecular semiconductors. <i>Physical Review B, 2018, 97,</i>	3.3	29
199	Machine learning of correlated dihedral potentials for atomistic molecular force fields. <i>Scientific Reports, 2018, 8, 2559</i>	4.9	17

198	Built-In Potentials Induced by Molecular Order in Amorphous Organic Thin Films. <i>ACS Applied Materials & Interfaces</i> , 2018 , 10, 1881-1887	9.5	40
197	Switching the Proton Conduction in Nanoporous, Crystalline Materials by Light. <i>Advanced Materials</i> , 2018 , 30, 1706551	24	78
196	Experimental characterization and simulation of amino acid and peptide interactions with inorganic materials. <i>Engineering in Life Sciences</i> , 2018 , 18, 84-100	3.4	16
195	Wavelength-Gated Dynamic Covalent Chemistry. <i>Angewandte Chemie - International Edition</i> , 2018 , 57, 2036-2045	16.4	83
194	Visible Light [2 + 2] Cycloadditions for Reversible Polymer Ligation. <i>Macromolecules</i> , 2018 , 51, 3802-3807	5.5	61
193	Meltdown! Local Heating by Decaying Excited Host Positive Polarons Triggers Aggregation Quenching in Blue PhOLEDs. <i>ChemPhysChem</i> , 2018 , 19, 2961-2966	3.2	6
192	26-4: Computer-Aided Optimization of Multilayer OLED Devices. <i>Digest of Technical Papers SID International Symposium</i> , 2018 , 49, 340-342	0.5	9
191	Anisotropic energy transfer in crystalline chromophore assemblies. <i>Nature Communications</i> , 2018 , 9, 4332	17.4	35
190	Photochemistry in Confined Environments for Single-Chain Nanoparticle Design. <i>Journal of the American Chemical Society</i> , 2018 , 140, 9551-9557	16.4	57
189	Effects of hydrogen ion irradiation on zinc oxide etching. <i>Journal of Vacuum Science and Technology A: Vacuum, Surfaces and Films</i> , 2017 , 35, 05C303	2.9	10
188	Effects of energy correlations and superexchange on charge transport and exciton formation in amorphous molecular semiconductors: An ab initio study. <i>Physical Review B</i> , 2017 , 95,	3.3	25
187	p-Doping of polystyrene polymers with attached functional side-groups from solution. <i>Journal of Materials Chemistry C</i> , 2017 , 5, 770-776	7.1	11
186	Generalized Born implicit solvent models for small molecule hydration free energies. <i>Physical Chemistry Chemical Physics</i> , 2017 , 19, 1677-1685	3.6	9
185	Molecular Origin of the Anisotropic Dye Orientation in Emissive Layers of Organic Light Emitting Diodes. <i>Chemistry of Materials</i> , 2017 , 29, 9528-9535	9.6	27
184	Structural origins of the cohesive energy in metal-terpyridine oligomer thin-films. <i>Physical Chemistry Chemical Physics</i> , 2017 , 19, 27952-27959	3.6	2
183	Binding patterns of homo-peptides on bare magnetic nanoparticles: insights into environmental dependence. <i>Scientific Reports</i> , 2017 , 7, 14047	4.9	17
182	Rational In Silico Design of an Organic Semiconductor with Improved Electron Mobility. <i>Advanced Materials</i> , 2017 , 29, 1703505	24	23
181	Charge-Transfer-Induced Lattice Collapse in Ni-Rich NCM Cathode Materials during Delithiation. <i>Journal of Physical Chemistry C</i> , 2017 , 121, 24381-24388	3.8	148

180	Anti-inflammatory effect of active nanofibrous polymeric membrane bearing nanocontainers of atorvastatin complexes. <i>Nanomedicine</i> , 2017 , 12, 2651-2674	5.6	11
179	Sub-50 nm Channel Vertical Field-Effect Transistors using Conventional Ink-Jet Printing. <i>Advanced Materials</i> , 2017 , 29, 1603858	24	23
178	Characterizing single chain nanoparticles (SCNPs): a critical survey. <i>Polymer Chemistry</i> , 2017 , 8, 5845-5854.	9	38
177	Ab initio charge-carrier mobility model for amorphous molecular semiconductors. <i>Physical Review B</i> , 2016 , 93,	3.3	38
176	Multiscale Simulation of Organic Electronics Via Smart Scheduling of Quantum Mechanics Computations. <i>Procedia Computer Science</i> , 2016 , 80, 1244-1254	1.6	2
175	Ultrarobust Thin-Film Devices from Self-Assembled Metal-Terpyridine Oligomers. <i>Advanced Materials</i> , 2016 , 28, 3473-80	24	21
174	Ligand-lipid and ligand-core affinity control the interaction of gold nanoparticles with artificial lipid bilayers and cell membranes. <i>Nanomedicine: Nanotechnology, Biology, and Medicine</i> , 2016 , 12, 1409-19	6	15
173	Chiral Porous Metacrystals: Employing Liquid-Phase Epitaxy to Assemble Enantiopure Metal-Organic Nanoclusters into Molecular Framework Pores. <i>ACS Nano</i> , 2016 , 10, 977-83	16.7	71
172	Biodegradable nanoparticles encapsulated in surface mounted metal-organic framework thin films. <i>Nanoscale</i> , 2016 , 8, 6468-72	7.7	22
171	Mechanisms of Nanoglass Ultrastability. <i>ACS Nano</i> , 2016 , 10, 3241-7	16.7	38
170	Concomitant partial exon skipping by a unique missense mutation of RPS6KA3 causes Coffin-Lowry syndrome. <i>Gene</i> , 2016 , 575, 42-7	3.8	7
169	Steric Clash in the SET Domain of Histone Methyltransferase NSD1 as a Cause of Sotos Syndrome and Its Genetic Heterogeneity in a Brazilian Cohort. <i>Genes</i> , 2016 , 7,	4.2	3
168	Molecular Origin of the Charge Carrier Mobility in Small Molecule Organic Semiconductors. <i>Advanced Functional Materials</i> , 2016 , 26, 5757-5763	15.6	62
167	Influence of Meso and Nanoscale Structure on the Properties of Highly Efficient Small Molecule Solar Cells. <i>Advanced Energy Materials</i> , 2016 , 6, 1501280	21.8	21
166	Molecular and Electronic Structure of the Cluster [Au ₈ (PPh ₃) ₈](NO ₃) ₂ . <i>European Journal of Inorganic Chemistry</i> , 2016 , 2016, 975-981	2.3	8
165	Superexchange Charge Transport in Loaded Metal Organic Frameworks. <i>ACS Nano</i> , 2016 , 10, 7085-93	16.7	48
164	Ab initio modeling of steady-state and time-dependent charge transport in hole-only OPD devices. <i>Applied Physics Letters</i> , 2016 , 109, 243301	3.4	11
163	Charge Transport by Superexchange in Molecular Host-Guest Systems. <i>Physical Review Letters</i> , 2016 , 117, 276803	7.4	32

162	QM/QM approach to model energy disorder in amorphous organic semiconductors. <i>Journal of Chemical Theory and Computation</i> , 2015 , 11, 560-7	6.4	32
161	Modelling of reversible single chain polymer self-assembly: from the polymer towards the protein limit. <i>Chemical Communications</i> , 2015 , 51, 6002-5	5.8	20
160	Toward Fast and Accurate Evaluation of Charge On-Site Energies and Transfer Integrals in Supramolecular Architectures Using Linear Constrained Density Functional Theory (CDFT)-Based Methods. <i>Journal of Chemical Theory and Computation</i> , 2015 , 11, 2077-86	6.4	34
159	Generalized effective-medium model for the carrier mobility in amorphous organic semiconductors. <i>Physical Review B</i> , 2015 , 91,	3.3	25
158	Experimental and theoretical study of phase separation in ZnPc:C60 blends. <i>Organic Electronics</i> , 2015 , 27, 183-191	3.5	4
157	Designing Molecular Printboards: A Photolithographic Platform for Recodable Surfaces. <i>Chemistry - A European Journal</i> , 2015 , 21, 13186-90	4.8	19
156	Band-gap engineering with a twist: Formation of intercalant superlattices in twisted graphene bilayers. <i>Physical Review B</i> , 2015 , 91,	3.3	17
155	Experimental and theoretical investigations of the electronic band structure of metal-organic frameworks of HKUST-1 type. <i>Applied Physics Letters</i> , 2015 , 107, 183301	3.4	52
154	Multiparticle moves in acceptance rate optimized Monte Carlo. <i>Journal of Computational Chemistry</i> , 2015 , 36, 2236-45	3.5	1
153	Charge carrier mobility and electronic properties of Al(Op) ₃ : impact of excimer formation. <i>Beilstein Journal of Nanotechnology</i> , 2015 , 6, 1107-15	3	6
152	Interfacial dominated ferromagnetism in nanograined ZnO: a BR and DFT study. <i>Scientific Reports</i> , 2015 , 5, 8871	4.9	92
151	Highly Selective Dispersion of Single-Walled Carbon Nanotubes via Polymer Wrapping: A Combinatorial Study via Modular Conjugation. <i>ACS Macro Letters</i> , 2014 , 3, 10-15	6.6	51
150	A fluorescence polarization assay for the experimental validation of an in silico model of the chemokine CXCL8 binding to receptor-derived peptides. <i>Physical Chemistry Chemical Physics</i> , 2014 , 16, 8036-43	3.6	9
149	Loading of ionic compounds into metal-organic frameworks: a joint theoretical and experimental study for the case of La ³⁺ . <i>Physical Chemistry Chemical Physics</i> , 2014 , 16, 17918-23	3.6	23
148	Ab Initio Treatment of Disorder Effects in Amorphous Organic Materials: Toward Parameter Free Materials Simulation. <i>Journal of Chemical Theory and Computation</i> , 2014 , 10, 3720-5	6.4	87
147	Spin-crossover and massive anisotropy switching of 5d transition metal atoms on graphene nanoflakes. <i>Nano Letters</i> , 2014 , 14, 3364-8	11.5	26
146	Cloning, functional characterization, and remodeling of K2P3.1 (TASK-1) potassium channels in a porcine model of atrial fibrillation and heart failure. <i>Heart Rhythm</i> , 2014 , 11, 1798-805	6.7	35
145	Structure of the membrane anchor of pestivirus glycoprotein E(rns), a long tilted amphipathic helix. <i>PLoS Pathogens</i> , 2014 , 10, e1003973	7.6	23

144	SLIM: an improved generalized Born implicit membrane model. <i>Journal of Computational Chemistry</i> , 2014 , 35, 2027-39	3.5	6
143	Cardiac expression and atrial fibrillation-associated remodeling of K β 2.1 (TREK-1) K ⁺ channels in a porcine model. <i>Life Sciences</i> , 2014 , 97, 107-15	6.8	30
142	Selective dispersion of large-diameter semiconducting single-walled carbon nanotubes with pyridine-containing copolymers. <i>Small</i> , 2014 , 10, 360-7	11	32
141	Six hydrophobins are involved in hydrophobin rodlet formation in <i>Aspergillus nidulans</i> and contribute to hydrophobicity of the spore surface. <i>PLoS ONE</i> , 2014 , 9, e94546	3.7	44
140	Calculation of the "absolute" free energy of a β hairpin in an all-atom force field. <i>Journal of Chemical Physics</i> , 2013 , 139, 054102	3.9	2
139	Thermodynamic Characterization of Protein Folding Equilibriums at the All Atom Level. <i>Biophysical Journal</i> , 2013 , 104, 369a-370a	2.9	
138	Structure based design of protein linkers for zinc finger nuclease. <i>FEBS Letters</i> , 2013 , 587, 3231-5	3.8	11
137	(4,4')-Bipyridine in vacuo and in solvents: a quantum chemical study of a prototypical floppy molecule from a molecular transport perspective. <i>Physical Chemistry Chemical Physics</i> , 2013 , 15, 1918-28 ^{3.6}		30
136	Folding and self-assembly of the TatA translocation pore based on a charge zipper mechanism. <i>Cell</i> , 2013 , 152, 316-26	56.2	52
135	[Au ₁₄ (PPh ₃) ₈ (NO ₃) ₄]: an example of a new class of Au(NO ₃)-ligated superatom complexes. <i>Angewandte Chemie - International Edition</i> , 2013 , 52, 3529-32	16.4	78
134	PowerBorn: A Barnes-Hut Tree Implementation for Accurate and Efficient Born Radii Computation. <i>Journal of Chemical Theory and Computation</i> , 2013 , 9, 1489-98	6.4	8
133	Catalytic subsurface etching of nanoscale channels in graphite. <i>Nature Communications</i> , 2013 , 4, 1379	17.4	40
132	Differential hERG ion channel activity of ultrasmall gold nanoparticles. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2013 , 110, 8004-9	11.5	53
131	Modeling disordered morphologies in organic semiconductors. <i>Journal of Computational Chemistry</i> , 2013 , 34, 2716-25	3.5	47
130	Magnetic anisotropy of graphene quantum dots decorated with a ruthenium adatom. <i>Beilstein Journal of Nanotechnology</i> , 2013 , 4, 441-5	3	3
129	Peptide structure prediction using distributed volunteer computing networks. <i>Journal of Mathematical Chemistry</i> , 2012 , 50, 421-428	2.1	4
128	In silico discovery of a compound with nanomolar affinity to antithrombin causing partial activation and increased heparin affinity. <i>Journal of Medicinal Chemistry</i> , 2012 , 55, 6403-12	8.3	43
127	Mirror images as naturally competing conformations in protein folding. <i>Journal of Physical Chemistry B</i> , 2012 , 116, 6880-8	3.4	30

126	7-Alkyl-3-benzylcoumarins: a versatile scaffold for the development of potent and selective cannabinoid receptor agonists and antagonists. <i>Journal of Medicinal Chemistry</i> , 2012 , 55, 7967-77	8.3	28
125	Modeling loop backbone flexibility in receptor-ligand docking simulations. <i>Journal of Computational Chemistry</i> , 2012 , 33, 2504-15	3.5	14
124	SIMONA 1.0: an efficient and versatile framework for stochastic simulations of molecular and nanoscale systems. <i>Journal of Computational Chemistry</i> , 2012 , 33, 2602-13	3.5	21
123	Different interface orientations of pentacene and PTCDA induce different degrees of disorder. <i>Nanoscale Research Letters</i> , 2012 , 7, 248	5	9
122	A peptidic unconjugated GRP78/BiP ligand modulates the unfolded protein response and induces prostate cancer cell death. <i>PLoS ONE</i> , 2012 , 7, e45690	3.7	28
121	Engineering hydrophobin DewA to generate surfaces that enhance adhesion of human but not bacterial cells. <i>Acta Biomaterialia</i> , 2012 , 8, 1037-47	10.8	28
120	Memory effects in electrochemically gated metallic point contacts. <i>Applied Physics Letters</i> , 2012 , 100, 203511	3.4	9
119	Selective dispersion of single-walled carbon nanotubes with specific chiral indices by poly(N-decyl-2,7-carbazole). <i>Journal of the American Chemical Society</i> , 2011 , 133, 652-5	16.4	126
118	Post-synthetic modification of epitaxially grown, highly oriented functionalized MOF thin films. <i>Chemical Communications</i> , 2011 , 47, 11210-2	5.8	52
117	Nasal embryonic LHRH factor (NELF) mutations in patients with normosmic hypogonadotropic hypogonadism and Kallmann syndrome. <i>Fertility and Sterility</i> , 2011 , 95, 1613-20.e1-7	4.8	50
116	Structural model of the gas vesicle protein GvpA and analysis of GvpA mutants in vivo. <i>Molecular Microbiology</i> , 2011 , 81, 56-68	4.1	32
115	Unique phenotype in a patient with CHARGE syndrome. <i>International Journal of Pediatric Endocrinology (Springer)</i> , 2011 , 2011, 11	1.5	8
114	Loading of Two Related Metal-Organic Frameworks (MOFs), [Cu ₂ (bdc) ₂ (dabco)] and [Cu ₂ (ndc) ₂ (dabco)], with Ferrocene. <i>Polymers</i> , 2011 , 3, 1565-1574	4.5	22
113	Receptor flexibility in small-molecule docking calculations. <i>Wiley Interdisciplinary Reviews: Computational Molecular Science</i> , 2011 , 1, 298-314	7.9	38
112	hERG K ⁺ channel-associated cardiac effects of the antidepressant drug desipramine. <i>Naunyn-Schmiedeberg's Archives of Pharmacology</i> , 2011 , 383, 119-39	3.4	34
111	Derivatives of molecular surface area and volume: simple and exact analytical formulas. <i>Journal of Computational Chemistry</i> , 2011 , 32, 2647-53	3.5	28
110	Branched DNA That Forms a Solid at 95 °C. <i>Angewandte Chemie</i> , 2011 , 123, 3285-3289	3.6	20
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