Clemence Corminboeuf

List of Publications by Year in Descending Order

130 papers	4,196 citations	35 h-index	60 g-index
146 ext. papers	5,072 ext. citations	7.4 avg, IF	6.31 L-index

#	Paper	IF	Citations
130	Heteroatom oxidation controls singlet-triplet energy splitting in singlet fission building blocks.. *Chemical Communications*, **2022**,	5.8	2
129	Uncovering the Activity of Alkaline Earth Metal Hydrogenation Catalysis Through Molecular Volcano Plots.. *Topics in Catalysis*, **2022**, 65, 289-295	2.3	0
128	Local Kernel Regression and Neural Network Approaches to the Conformational Landscapes of Oligopeptides.. *Journal of Chemical Theory and Computation*, **2022**, 18, 1467-1479	6.4	1
127	Assessing the persistence of chalcogen bonds in solution with neural network potentials.. *Journal of Chemical Physics*, **2022**, 156, 154112	3.9	1
126	Optimizing the Thermodynamics and Kinetics of the Triplet-Pair Dissociation in Donor-Acceptor Copolymers for Intramolecular Singlet Fission.. *Chemistry of Materials*, **2022**, 34, 4115-4121	9.6	2
125	Identifying the Trade-off between Intramolecular Singlet Fission Requirements in Donor□Acceptor Copolymers. *Chemistry of Materials*, **2021**, 33, 2567-2575	9.6	5
124	Learning the Exciton Properties of Azo-dyes. *Journal of Physical Chemistry Letters*, **2021**, 12, 5957-5962	6.4	0
123	Impact of quantum-chemical metrics on the machine learning prediction of electron density. *Journal of Chemical Physics*, **2021**, 155, 024107	3.9	2
122	Tuning the □Accepting Properties of Mesoionic Carbenes: A Combined Computational and Experimental Study. *Chemistry - A European Journal*, **2021**, 27, 11983-11988	4.8	2
121	Pushing the Limits of the Donor-Acceptor Copolymer Strategy for Intramolecular Singlet Fission. *Journal of Physical Chemistry Letters*, **2021**, 12, 7270-7277	6.4	3
120	Structure-Property Relationships in Bithiophenes with Hydrogen-Bonded Substituents. *Chemistry - A European Journal*, **2021**, 27, 3348-3360	4.8	5
119	Helical electronic transitions of spiroconjugated molecules. *Chemical Communications*, **2021**, 57, 6408-6418	5.8	6
118	The Genesis of Molecular Volcano Plots. *Accounts of Chemical Research*, **2021**, 54, 1107-1117	24.3	17
117	Is a Single Conformer Sufficient to Describe the Reorganization Energy of Amorphous Organic Transport Materials?. *Journal of Physical Chemistry C*, **2021**, 125, 17355-17362	3.8	2
116	Reaction-based machine learning representations for predicting the enantioselectivity of organocatalysts. *Chemical Science*, **2021**, 12, 6879-6889	9.4	15
115	Tuning the Thermal Stability and Photoisomerization of Azoheteroarenes through Macrocycle Strain*. *Chemistry - A European Journal*, **2021**, 27, 419-426	4.8	6
114	FB-ECDA: Fragment-based Electronic Coupling Decomposition Analysis for Organic Amorphous Semiconductors. *Journal of Physical Chemistry A*, **2020**, 124, 10624-10634	2.8	1

113	Direct, Mediated, and Delayed Intramolecular Singlet Fission Mechanism in Donor-Acceptor Copolymers. *Journal of Physical Chemistry Letters*, **2020**, 11, 9788-9794	6.4	7
112	Learning (from) the Electron Density: Transferability, Conformational and Chemical Diversity. *Chimia*, **2020**, 74, 232-236	1.3	6
111	Machine learning models of the energy curvature vs particle number for optimal tuning of long-range corrected functionals. *Journal of Chemical Physics*, **2020**, 152, 154103	3.9	7
110	FB-REDA: fragment-based decomposition analysis of the reorganization energy for organic semiconductors. *Physical Chemistry Chemical Physics*, **2020**, 22, 11881-11890	3.6	7
109	Data-Driven Advancement of Homogeneous Nickel Catalyst Activity for Aryl Ether Cleavage. *ACS Catalysis*, **2020**, 10, 7021-7031	13.1	17
108	Simulating Solvation and Acidity in Complex Mixtures with First-Principles Accuracy: The Case of CHSOH and HO in Phenol. *Journal of Chemical Theory and Computation*, **2020**, 16, 5139-5149	6.4	15
107	Hamiltonian-Reservoir Replica Exchange and Machine Learning Potentials for Computational Organic Chemistry. *Journal of Chemical Theory and Computation*, **2020**, 16, 3084-3094	6.4	8
106	Crystallization and Organic Field-Effect Transistor Performance of a Hydrogen-Bonded Quaterthiophene. *Chemistry - A European Journal*, **2020**, 26, 10265-10275	4.8	4
105	Balancing Density Functional Theory Interaction Energies in Charged Dimers Precursors to Organic Semiconductors. *Journal of Chemical Theory and Computation*, **2020**, 16, 3530-3542	6.4	2
104	Correlation between Optical Activity and the Helical Molecular Orbitals of Allene and Cumulenes. *Organic Letters*, **2020**, 22, 8028-8033	6.2	5
103	Learning on-top: Regressing the on-top pair density for real-space visualization of electron correlation. *Journal of Chemical Physics*, **2020**, 153, 204111	3.9	9
102	Doped but Stable: Spirobisacridine Hole Transporting Materials for Hysteresis-Free and Stable Perovskite Solar Cells. *Journal of the American Chemical Society*, **2020**, 142, 1792-1800	16.4	29
101	Data-powered augmented volcano plots for homogeneous catalysis. *Chemical Science*, **2020**, 11, 12070-12080	9.4	14
100	The Photoisomerization Pathway(s) of Push-Pull Phenylazoheteroarenes*. *Chemistry - A European Journal*, **2020**, 26, 14724-14729	4.8	3
99	Designing Singlet Fission Candidates from Donor-Acceptor Copolymers. *Chemistry of Materials*, **2020**, 32, 6515-6524	9.6	16
98	Optical gap and fundamental gap of oligoynes and carbyne. *Nature Communications*, **2020**, 11, 4797	17.4	13
97	Probing Substrate Scope with Molecular Volcanoes. *Organic Letters*, **2020**, 22, 7936-7941	6.2	6
96	Optical absorption properties of metal-organic frameworks: solid state molecular perspective. *Physical Chemistry Chemical Physics*, **2020**, 22, 19512-19521	3.6	8

95	Direct Observation of Aggregation-Induced Emission Mechanism. *Angewandte Chemie*, **2020**, 132, 15013-15019	3.6	5
94	Direct Observation of Aggregation-Induced Emission Mechanism. *Angewandte Chemie - International Edition*, **2020**, 59, 14903-14909	16.4	44
93	Exploring chemical space in the search for improved azoheteroarene-based photoswitches. *Physical Chemistry Chemical Physics*, **2019**, 21, 20782-20790	3.6	8
92	Electron density learning of non-covalent systems. *Chemical Science*, **2019**, 10, 9424-9432	9.4	55
91	Insights into Reaction Intermediates to Predict Synthetic Pathways for Shape-Controlled Metal Nanocrystals. *Journal of the American Chemical Society*, **2019**, 141, 16312-16322	16.4	29
90	The influence of external electric fields on charge reorganization energy in organic semiconductors. *Chemical Communications*, **2019**, 55, 2384-2387	5.8	6
89	Topology-Driven Single-Molecule Conductance of Carbon Nanothreads. *Journal of Physical Chemistry Letters*, **2019**, 10, 825-830	6.4	13
88	Synthesis of aminyl biradicals by base-induced Csp-Csp coupling of cationic azo dyes. *Chemical Science*, **2019**, 10, 5719-5724	9.4	20
87	Activity-Based Screening of Homogeneous Catalysts through the Rapid Assessment of Theoretically Derived Turnover Frequencies. *ACS Catalysis*, **2019**, 9, 5716-5725	13.1	24
86	Data Mining the C□ Cross-Coupling Genome. *ChemCatChem*, **2019**, 11, 4096-4107	5.2	10
85	DORI Reveals the Influence of Noncovalent Interactions on Covalent Bonding Patterns in Molecular Crystals Under Pressure. *Journal of Physical Chemistry Letters*, **2019**, 10, 1482-1488	6.4	9
84	Mechanisms of fluorescence quenching in prototypical aggregation-induced emission systems: excited state dynamics with TD-DFTB. *Physical Chemistry Chemical Physics*, **2019**, 21, 9026-9035	3.6	19
83	An Unconventional Iron Nickel Catalyst for the Oxygen Evolution Reaction. *ACS Central Science*, **2019**, 5, 558-568	16.8	136
82	Tuning the structure, reactivity and magnetic communication of nitride-bridged uranium complexes with the ancillary ligands. *Chemical Science*, **2019**, 10, 8840-8849	9.4	16
81	Open-Shell Nonbenzenoid Nanographenes Containing Two Pairs of Pentagonal and Heptagonal Rings. *Journal of the American Chemical Society*, **2019**, 141, 12011-12020	16.4	47
80	Dual-Facet Mechanism in Copper Nanocubes for Electrochemical CO Reduction into Ethylene. *Journal of Physical Chemistry Letters*, **2019**, 10, 4259-4265	6.4	30
79	Mechanistic Study on the Photogeneration of Hydrogen by Decamethylruthenocene. *Chemistry - A European Journal*, **2019**, 25, 12769-12779	4.8	4
78	Getting the Right Twist: Influence of Donor□Acceptor Dihedral Angle on Exciton Kinetics and Singlet□Triplet Gap in Deep Blue Thermally Activated Delayed Fluorescence Emitter. *Journal of Physical Chemistry C*, **2019**, 123, 27778-27784	3.8	23

77	Multiarm and Substituent Effects on Charge Transport of Organic Hole Transport Materials. *Chemistry of Materials*, **2019**, 31, 6605-6614	9.6	15
76	Quantum Chemistry Meets Machine Learning. *Chimia*, **2019**, 73, 983-989	1.3	6
75	Transferable Machine-Learning Model of the Electron Density. *ACS Central Science*, **2019**, 5, 57-64	16.8	114
74	The role of bridging ligands in dinitrogen reduction and functionalization by uranium multimetallic complexes. *Nature Chemistry*, **2019**, 11, 154-160	17.6	67
73	i-PI 2.0: A universal force engine for advanced molecular simulations. *Computer Physics Communications*, **2019**, 236, 214-223	4.2	118
72	Noncovalent Molecular Electronics. *Journal of Physical Chemistry Letters*, **2018**, 9, 2298-2304	6.4	10
71	How does alkyl chain length modify the properties of triphenylamine-based hole transport materials?. *Journal of Materials Chemistry C*, **2018**, 6, 960-965	7.1	19
70	How do London Dispersion Interactions Impact the Photochemical Processes of Molecular Switches?. *Journal of Physical Chemistry Letters*, **2018**, 9, 464-470	6.4	16
69	Analyzing Fluxional Molecules Using DORI. *Journal of Chemical Theory and Computation*, **2018**, 14, 2370-2379	5.4	5
68	Expedited Screening of Active and Regioselective Catalysts for the Hydroformylation Reaction. *Helvetica Chimica Acta*, **2018**, 101, e1800107	2	15
67	Machine learning meets volcano plots: computational discovery of cross-coupling catalysts. *Chemical Science*, **2018**, 9, 7069-7077	9.4	118
66	Steric "attraction": not by dispersion alone. *Beilstein Journal of Organic Chemistry*, **2018**, 14, 1482-1490	2.5	14
65	Improving the Thermodynamic Profiles of Prospective Suzuki–Miyaura Cross-Coupling Catalysts by Altering the Electrophilic Coupling Component. *ChemCatChem*, **2018**, 10, 1592-1597	5.2	15
64	On the Generality of Molecular Volcano Plots. *ChemCatChem*, **2018**, 10, 1586-1591	5.2	20
63	Unraveling Metal/Pincer Ligand Effects in the Catalytic Hydrogenation of Carbon Dioxide to Formate. *Organometallics*, **2018**, 37, 4568-4575	3.8	18
62	Restriction Enzyme Analysis of Double-Stranded DNA on Pristine Single-Walled Carbon Nanotubes. *ACS Applied Materials & Interfaces*, **2018**, 10, 37386-37395	9.5	7
61	Read between the Molecules: Computational Insights into Organic Semiconductors. *Journal of the American Chemical Society*, **2018**, 140, 16370-16386	16.4	58
60	Exploring the Limitation of Molecular Water Oxidation Catalysts. *Journal of Physical Chemistry C*, **2018**, 122, 12404-12412	3.8	27

59	Fine-tuned organic photoredox catalysts for fragmentation-alkynylation cascades of cyclic oxime ethers. *Chemical Science*, **2018**, 9, 5883-5889	9.4	117
58	Infrared Spectroscopy as a Probe of Electronic Energy Transfer. *Journal of Physical Chemistry Letters*, **2018**, 9, 3217-3223	6.4	8
57	Nickel pincer model of the active site of lactate racemase involves ligand participation in hydride transfer. *Proceedings of the National Academy of Sciences of the United States of America*, **2017**, 114, 1242-1245	11.5	30
56	Enhancing the power conversion efficiency of dye-sensitized solar cells via molecular plasmon-like excitations. *Chemical Communications*, **2017**, 53, 2423-2426	5.8	4
55	Photoproduction of Hydrogen by Decamethylruthenocene Combined with Electrochemical Recycling. *Angewandte Chemie - International Edition*, **2017**, 56, 2324-2327	16.4	18
54	Photoproduction of Hydrogen by Decamethylruthenocene Combined with Electrochemical Recycling. *Angewandte Chemie*, **2017**, 129, 2364-2367	3.6	5
53	Synthesis and characterization of semiaromatic polyamides comprising benzofurobenzofuran repeating units. *Polymer Chemistry*, **2017**, 8, 2197-2209	4.9	10
52	Heterotetracenes: Flexible Synthesis and in Silico Assessment of the Hole-Transport Properties. *Chemistry - A European Journal*, **2017**, 23, 8058-8065	4.8	21
51	Fluorescence Quenching in BODIPY Dyes: The Role of Intramolecular Interactions and Charge Transfer. *Helvetica Chimica Acta*, **2017**, 100, e1700093	2	26
50	Perspective: Found in translation: Quantum chemical tools for grasping non-covalent interactions. *Journal of Chemical Physics*, **2017**, 146, 120901	3.9	65
49	Charge transport in highly ordered organic nanofibrils: lessons from modelling. *Journal of Materials Chemistry C*, **2017**, 5, 350-361	7.1	17
48	Salt-induced thermochromism of a conjugated polyelectrolyte. *Physical Chemistry Chemical Physics*, **2017**, 19, 28853-28866	3.6	8
47	A Carbon elimination strategy for convenient access to cyclopentadienyl metal complexes. *Chemical Science*, **2017**, 8, 7174-7179	9.4	37
46	A Rising Star: Truxene as a Promising Hole Transport Material in Perovskite Solar Cells. *Journal of Physical Chemistry C*, **2017**, 121, 21729-21739	3.8	23
45	A Generalized Picture of C Cross-Coupling. *ACS Catalysis*, **2017**, 7, 5643-5653	13.1	55
44	Guidelines and diagnostics for charge carrier tuning in thiophene-based wires. *Physical Chemistry Chemical Physics*, **2017**, 19, 23254-23259	3.6	10
43	Photochromic Torsional Switch (PTS): a light-driven actuator for the dynamic tuning of conjugation extension. *Chemical Science*, **2017**, 8, 361-365	9.4	11
42	How does tetraphenylethylene relax from its excited states?. *Physical Chemistry Chemical Physics*, **2016**, 18, 11606-9	3.6	76

41	Rationalizing fluorescence quenching in meso-BODIPY dyes. *Physical Chemistry Chemical Physics*, **2016**, 18, 32668-32672	3.6	36
40	Neutral Aminyl Radicals Derived from Azoimidazolium Dyes. *Journal of the American Chemical Society*, **2016**, 138, 15126-15129	16.4	32
39	Visualizing and Quantifying Interactions in the Excited State. *Chemistry - A European Journal*, **2016**, 22, 18442-18449	4.8	21
38	Accessing and predicting the kinetic profiles of homogeneous catalysts from volcano plots. *Chemical Science*, **2016**, 7, 5723-5735	9.4	44
37	Beyond static structures: Putting forth REMD as a tool to solve problems in computational organic chemistry. *Journal of Computational Chemistry*, **2016**, 37, 83-92	3.5	21
36	Implications of Charge Penetration for Heteroatom-Containing Organic Semiconductors. *Journal of Physical Chemistry Letters*, **2016**, 7, 5198-5204	6.4	25
35	Low-Lying π States of Heteroaromatic Molecules: A Challenge for Excited State Methods. *Journal of Chemical Theory and Computation*, **2016**, 12, 2652-60	6.4	47
34	Communication: A new class of non-empirical explicit density functionals on the third rung of Jacob's ladder. *Journal of Chemical Physics*, **2015**, 143, 111105	3.9	13
33	Local hybrid functionals with orbital-free mixing functions and balanced elimination of self-interaction error. *Journal of Chemical Physics*, **2015**, 142, 074112	3.9	26
32	Excited state dynamics of thiophene and bithiophene: new insights into theoretically challenging systems. *Physical Chemistry Chemical Physics*, **2015**, 17, 14719-30	3.6	44
31	Linear scaling relationships and volcano plots in homogeneous catalysis - revisiting the Suzuki reaction. *Chemical Science*, **2015**, 6, 6754-6761	9.4	68
30	Exploiting Dispersion-Driven Aggregators as a Route to New One-Dimensional Organic Nanowires. *Journal of Physical Chemistry Letters*, **2015**, 6, 4422-8	6.4	10
29	Theory and practice of uncommon molecular electronic configurations. *Wiley Interdisciplinary Reviews: Computational Molecular Science*, **2015**, 5, 440-459	7.9	66
28	Intramolecular symmetry-adapted perturbation theory with a single-determinant wavefunction. *Journal of Chemical Physics*, **2015**, 143, 224107	3.9	16
27	A fast charge-Dependent atom-pairwise dispersion correction for DFTB3. *International Journal of Quantum Chemistry*, **2015**, 115, 1265-1272	2.1	16
26	Toward functional type III [Fe]-hydrogenase biomimics for H2 activation: insights from computation. *Chemistry - A European Journal*, **2015**, 21, 3987-96	4.8	19
25	Functional carbon nanosheets prepared from hexayne amphiphile monolayers at room temperature. *Nature Chemistry*, **2014**, 6, 468-76	17.6	85
24	Adjusting the Local Arrangement of π-Stacked Oligothiophenes through Hydrogen Bonds: A Viable Route to Promote Charge Transfer. *Journal of Physical Chemistry Letters*, **2014**, 5, 2320-4	6.4	21

23	Ligand-controlled regiodivergent pathways of rhodium(III)-catalyzed dihydroisoquinolone synthesis: experimental and computational studies of different cyclopentadienyl ligands. *Chemistry - A European Journal*, **2014**, 20, 15409-18	4.8	100
22	Simultaneous Visualization of Covalent and Noncovalent Interactions Using Regions of Density Overlap. *Journal of Chemical Theory and Computation*, **2014**, 10, 3745-3756	6.4	132
21	Minimizing density functional failures for non-covalent interactions beyond van der Waals complexes. *Accounts of Chemical Research*, **2014**, 47, 3217-24	24.3	45
20	Exploration of zeroth-order wavefunctions and energies as a first step toward intramolecular symmetry-adapted perturbation theory. *Journal of Chemical Physics*, **2014**, 140, 154107	3.9	14
19	How important is self-consistency for the dDsC density dependent dispersion correction?. *Journal of Chemical Physics*, **2014**, 140, 18A516	3.9	23
18	Hierarchically structured microfibers of "single stack" perylene bisimide and quaterthiophene nanowires. *ACS Nano*, **2013**, 7, 8498-508	16.7	78
17	A ratiometric fluorescence sensor for caffeine. *Organic and Biomolecular Chemistry*, **2012**, 10, 7487-90	3.9	18
16	Biphasic water splitting by osmocene. *Proceedings of the National Academy of Sciences of the United States of America*, **2012**, 109, 11558-63	11.5	38
15	Exploring the Limits of Density Functional Approximations for Interaction Energies of Molecular Precursors to Organic Electronics. *Journal of Chemical Theory and Computation*, **2012**, 8, 4305-16	6.4	34
14	Quantification of "fuzzy" chemical concepts: a computational perspective. *Chemical Society Reviews* , **2012**, 41, 4671-87	58.5	88
13	Why are the Interaction Energies of Charge-Transfer Complexes Challenging for DFT?. *Journal of Chemical Theory and Computation*, **2012**, 8, 1629-40	6.4	141
12	Comprehensive Benchmarking of a Density-Dependent Dispersion Correction. *Journal of Chemical Theory and Computation*, **2011**, 7, 3567-77	6.4	322
11	A density dependent dispersion correction. *Chimia*, **2011**, 65, 240-4	1.3	35
10	Dispersion-corrected energy decomposition analysis for intermolecular interactions based on the BLW and dDXDM methods. *Journal of Physical Chemistry A*, **2011**, 115, 5467-77	2.8	38
9	A generalized-gradient approximation exchange hole model for dispersion coefficients. *Journal of Chemical Physics*, **2011**, 134, 044117	3.9	211
8	A System-Dependent Density-Based Dispersion Correction. *Journal of Chemical Theory and Computation*, **2010**, 6, 1990-2001	6.4	118
7	Why Are (NN2)Ni Pincer Complexes Active for Alkyl–Alkyl Coupling: β-H Elimination Is Kinetically Accessible but Thermodynamically Uphill. *Organometallics*, **2010**, 29, 3686-3689	3.8	73
6	Oxygen and proton reduction by decamethylferrocene in non-aqueous acidic media. *Chemical Communications*, **2010**, 46, 2918-9	5.8	51

5	Unified Inter- and Intramolecular Dispersion Correction Formula for Generalized Gradient Approximation Density Functional Theory. *Journal of Chemical Theory and Computation*, **2009**, 5, 2950-8	6.4	70
4	Can five-membered Te2N2S rings be considered aromatic?. *Structural Chemistry*, **2007**, 18, 841-847	1.8	3
3	Methoxycyclization of 1,5-Enynes by Coinage Metal Catalysts: Is Gold Always Superior?. *Helvetica Chimica Acta*,e2100134	2	0
2	Machine intelligence for chemical reaction space. *Wiley Interdisciplinary Reviews: Computational Molecular Science*,	7.9	2
1	Donor□Acceptor□Donor □Hot Exciton□Triads for High Reverse Intersystem Crossing in OLEDs. *Advanced Optical Materials*,2200509	8.1	0