Toon Verstraelen

List of Publications by Year in descending order

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69 papers	4,027 citations	147726 31 h-index	118793 62 g-index
72 all docs	72 docs citations	72 times ranked	4437 citing authors

#	Article	IF	Citations
1	The ReaxFF reactive force-field: development, applications and future directions. Npj Computational Materials, 2016, 2, .	3.5	1,319
2	TAMkin: A Versatile Package for Vibrational Analysis and Chemical Kinetics. Journal of Chemical Information and Modeling, 2010, 50, 1736-1750.	2.5	155
3	QuickFF: A program for a quick and easy derivation of force fields for metalâ€organic frameworks from ab initio input. Journal of Computational Chemistry, 2015, 36, 1015-1027.	1.5	132
4	Metalâ€“organic frameworks as potential shock absorbers: the case of the highly flexible MIL-53(Al). Chemical Communications, 2014, 50, 9462-9464.	2.2	122
5	Minimal Basis Iterative Stockholder: Atoms in Molecules for Force-Field Development. Journal of Chemical Theory and Computation, 2016, 12, 3894-3912.	2.3	119
6	Thermodynamic Insight in the High-Pressure Behavior of UiO-66: Effect of Linker Defects and Linker Expansion. Chemistry of Materials, 2016, 28, 5721-5732.	3.2	97
7	Information-Theoretic Approaches to Atoms-in-Molecules: Hirshfeld Family of Partitioning Schemes. Journal of Physical Chemistry A, 2018, 122, 4219-4245.	1.1	97
8	Vibrational modes in partially optimized molecular systems. Journal of Chemical Physics, 2007, 126, 224102.	1.2	95
9	eReaxFF: A Pseudoclassical Treatment of Explicit Electrons within Reactive Force Field Simulations. Journal of Chemical Theory and Computation, 2016, 12, 3463-3472.	2.3	91
10	ACKS2: Atom-condensed Kohn-Sham DFT approximated to second order. Journal of Chemical Physics, 2013, 138, 074108.	1.2	84
11	A Comparison of Barostats for the Mechanical Characterization of Metalâ€“Organic Frameworks. Journal of Chemical Theory and Computation, 2015, 11, 5583-5597.	2.3	83
12	The electronegativity equalization method and the split charge equilibration applied to organic systems: Parametrization, validation, and comparison. Journal of Chemical Physics, 2009, 131, 044127.	1.2	82
13	New Functionalized Metalâ€“Organic Frameworks MIL-47-X (X = â^'Cl, â^'Br, â^'CH₃,) Tj ETQq1 1 0.784314 rgBT /Overlock Adsorption Properties. Journal of Physical Chemistry C, 2013, 117, 22784-22796.	1.5	79
14	Hirshfeld-E Partitioning: AIM Charges with an Improved Trade-off between Robustness and Accurate Electrostatics. Journal of Chemical Theory and Computation, 2013, 9, 2221-2225.	2.3	77
15	Assessing the Accuracy of New Geminal-Based Approaches. Journal of Physical Chemistry A, 2014, 118, 9058-9068.	1.1	77
16	Ab Initio Parametrized Force Field for the Flexible Metalâ€“Organic Framework MIL-53(Al). Journal of Chemical Theory and Computation, 2012, 8, 3217-3231.	2.3	69
17	Assessment of Atomic Charge Models for Gas-Phase Computations on Polypeptides. Journal of Chemical Theory and Computation, 2012, 8, 661-676.	2.3	66
18	MFI Fingerprint: How Pentasil-Induced IR Bands Shift during Zeolite Nanogrowth. Journal of Physical Chemistry C, 2008, 112, 9186-9191.	1.5	59

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19	Extension of the QuickFF force field protocol for an improved accuracy of structural, vibrational, mechanical and thermal properties of metalâ€“organic frameworks. Journal of Computational Chemistry, 2018, 39, 999-1011.	1.5	59
20	Opposite Regiospecific Ring Opening of 2-(Cyanomethyl)aziridines by Hydrogen Bromide and Benzyl Bromide: Experimental Study and Theoretical Rationalization. Journal of Organic Chemistry, 2010, 75, 4530-4541.	1.7	56
21	ReaxFF Parameter Optimization with Monte-Carlo and Evolutionary Algorithms: Guidelines and Insights. Journal of Chemical Theory and Computation, 2019, 15, 6799-6812.	2.3	54
22	The Monomer Electron Density Force Field (MEDFF): A Physically Inspired Model for Noncovalent Interactions. Journal of Chemical Theory and Computation, 2017, 13, 161-179.	2.3	53
23	ZEOBUILDER: A GUI Toolkit for the Construction of Complex Molecular Structures on the Nanoscale with Building Blocks. Journal of Chemical Information and Modeling, 2008, 48, 1530-1541.	2.5	48
24	Computation of Charge Distribution and Electrostatic Potential in Silicates with the Use of Chemical Potential Equalization Models. Journal of Physical Chemistry C, 2012, 116, 490-504.	1.5	47
25	An explicit approach to conceptual density functional theory descriptors of arbitrary order. Chemical Physics Letters, 2016, 660, 307-312.	1.2	46
26	The Significance of Parameters in Charge Equilibration Models. Journal of Chemical Theory and Computation, 2011, 7, 1750-1764.	2.3	42
27	Automated Parametrization of AMBER Force Field Terms from Vibrational Analysis with a Focus on Functionalizing Dinuclear Zinc(II) Scaffolds. Journal of Chemical Theory and Computation, 2012, 8, 554-562.	2.3	42
28	Modeling Gas Adsorption in Flexible Metalâ€“Organic Frameworks via Hybrid Monte Carlo/Molecular Dynamics Schemes. Advanced Theory and Simulations, 2019, 2, 1800177.	1.3	40
29	When is the Fukui Function Not Normalized? The Danger of Inconsistent Energy Interpolation Models in Density Functional Theory. Journal of Chemical Theory and Computation, 2016, 12, 5777-5787.	2.3	38
30	Calculating Reaction Rates with Partial Hessians: Validation of the Mobile Block Hessian Approach. Journal of Chemical Theory and Computation, 2008, 4, 614-625.	2.3	35
31	The conformational sensitivity of iterative stockholder partitioning schemes. Chemical Physics Letters, 2012, 545, 138-143.	1.2	35
32	Methane Adsorption in Zr-Based MOFs: Comparison and Critical Evaluation of Force Fields. Journal of Physical Chemistry C, 2017, 121, 25309-25322.	1.5	34
33	Multi-level Modeling of Silicaâ€“Template Interactions During Initial Stages of Zeolite Synthesis. Topics in Catalysis, 2009, 52, 1261-1271.	1.3	31
34	Hydration Free Energies in the FreeSolv Database Calculated with Polarized Iterative Hirshfeld Charges. Journal of Chemical Information and Modeling, 2018, 58, 1779-1797.	2.5	31
35	Direct computation of parameters for accurate polarizable force fields. Journal of Chemical Physics, 2014, 141, 194114.	1.2	28
36	Ab initio calculation of entropy and heat capacity of gas-phase n-alkanes with hetero-elements O and S: Ethers/alcohols and sulfides/thiols. Chemical Physics, 2006, 328, 251-258.	0.9	25

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37	Hostâ€“guest and guestâ€“guest interactions between xylene isomers confined in the MIL-47(V) pore system. Theoretical Chemistry Accounts, 2012, 131, 1.	0.5	23
38	MD-TRACKS: A Productive Solution for the Advanced Analysis of Molecular Dynamics and Monte Carlo simulations. Journal of Chemical Information and Modeling, 2008, 48, 2414-2424.	2.5	21
39	Diphosphonylation of Aromatic Diazaheterocycles and Theoretical Rationalization of Product Yields. European Journal of Organic Chemistry, 2013, 2013, 1058-1067.	1.2	21
40	Charting the Complete Thermodynamic Landscape of Gas Adsorption for a Responsive Metalâ€“Organic Framework. Journal of the American Chemical Society, 2021, 143, 4143-4147.	6.6	21
41	Influence of Protein Environment on the Electron Paramagnetic Resonance Properties of Flavoprotein Radicals: A QM/MM Study. Journal of Physical Chemistry B, 2010, 114, 16655-16665.	1.2	20
42	Catalytic Performance of Vanadium MILâ€47 and Linkerâ€Substituted Variants in the Oxidation of Cyclohexene: A Combined Theoretical and Experimental Approach. ChemPlusChem, 2014, 79, 1183-1197.	1.3	20
43	The Gradient Curves Method:â€‰ An Improved Strategy for the Derivation of Molecular Mechanics Valence Force Fields from ab Initio Data. Journal of Chemical Theory and Computation, 2007, 3, 1420-1434.	2.3	19
44	Conformational Sampling of Macrocyclic Alkenes Using a Kennardâˆ’Stone-Based Algorithm. Journal of Physical Chemistry A, 2010, 114, 6879-6887.	1.1	17
45	<scp>IOData</scp>: A python library for reading, writing, and converting computational chemistry file formats and generating input files. Journal of Computational Chemistry, 2021, 42, 458-464.	1.5	17
46	Molecular dynamics study of the silicaâ€“waterâ€“SDA interactions. Physical Chemistry Chemical Physics, 2009, 11, 7605.	1.3	16
47	The Influence of Ser-154, Cys-113, and the Phosphorylated Threonine Residue on the Catalytic Reaction Mechanism of Pin1. Journal of Physical Chemistry B, 2014, 118, 9871-9880.	1.2	16
48	Super-ions of sodium cations with hydrated hydroxide anions: inorganic structure-directing agents in zeolite synthesis. Materials Horizons, 2021, 8, 2576-2583.	6.4	16
49	Temperature Study of a Glycine Radical in the Solid State Adopting a DFT Periodic Approach: Vibrational Analysis and Comparison with EPR Experiments. Journal of Physical Chemistry B, 2008, 112, 7618-7630.	1.2	15
50	Is the error on first-principles volume predictions absolute or relative?. Computational Materials Science, 2016, 117, 390-396.	1.4	15
51	Can the electronegativity equalization method predict spectroscopic properties?. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2015, 136, 76-80.	2.0	13
52	The local response of global descriptors. Theoretical Chemistry Accounts, 2017, 136, 1.	0.5	12
53	Ab Initio Evaluation of Henry Coefficients Using Importance Sampling. Journal of Chemical Theory and Computation, 2018, 14, 6359-6369.	2.3	12
54	Insight into the Solvation and Isomerization of 3â€Haloâ€1â€azaallylic Anions from Ab Initio Metadynamics Calculations and NMR Experiments. Chemistry - A European Journal, 2009, 15, 580-584.	1.7	10

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55	Atomic Velocity Projection Method: A New Analysis Method for Vibrational Spectra in Terms of Internal Coordinates for a Better Understanding of Zeolite Nanogrowth. Journal of Chemical Theory and Computation, 2011, 7, 1045-1061.	2.3	10
56	Modeling Electronic Response Properties with an Explicit-Electron Machine Learning Potential. Journal of Chemical Theory and Computation, 2022, 18, 1672-1691.	2.3	10
57	Exploring the substrate selectivity of human sEH and M. tuberculosis EHB using QM/MM. Structural Chemistry, 2017, 28, 1501-1511.	1.0	9
58	ParAMS: Parameter Optimization for Atomistic and Molecular Simulations. Journal of Chemical Information and Modeling, 2021, 61, 3737-3743.	2.5	9
59	Effect of temperature on the EPR properties of a rhamnose alkoxy radical: A DFT molecular dynamics study. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2008, 69, 1388-1394.	2.0	8
60	Critical Analysis of the Accuracy of Models Predicting or Extracting Liquid Structure Information. Journal of Physical Chemistry B, 2014, 118, 2451-2470.	1.2	5
61	Improving the Silicon Interactions of GFN-xTB. Journal of Chemical Information and Modeling, 2021, 61, 5931-5937.	2.5	5
62	Analysis of the basis set superposition error in molecular dynamics of hydrogen-bonded liquids: Application to methanol. Journal of Chemical Physics, 2012, 137, 104506.	1.2	4
63	Cationâ˜Ï€ Interactions Accelerate the Living Cationic Ring-Opening Polymerization of Unsaturated 2-Alkyl-2-oxazolines. Macromolecules, 2020, 53, 3832-3846.	2.2	4
64	Structure-aided optimization of non-nucleoside M.Âtuberculosis thymidylate kinase inhibitors. European Journal of Medicinal Chemistry, 2021, 225, 113784.	2.6	4
65	Multiscale partial charge estimation on graphene for neutral, doped and charged flakes. Physical Chemistry Chemical Physics, 2018, 20, 20678-20687.	1.3	2
66	Zeo-1, a computational data set of zeolite structures. Scientific Data, 2022, 9, 61.	2.4	2
67	Constrained iterative Hirshfeld charges: A variational approach. Journal of Chemical Physics, 2022, 156, .	1.2	2
68	GloMPO (Globally Managed Parallel Optimization): a tool for expensive, black-box optimizations, application to ReaxFF reparameterizations. Journal of Cheminformatics, 2022, 14, 7.	2.8	1
69	Reparameterization ofÂComputational Chemistry Force Fields Using GloMPO (Globally Managed) Tj ETQq1 1 0.784314 rgBT /Overloc	1.0	0