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	Modeling Electronic Response Properties with an Explicit-Electron Machine Learning Potential. Journal of Chemical Theory and Computation, 2022, 18, 1672-1691.	2.3	10
2	Zeo-1, a computational data set of zeolite structures. Scientific Data, 2022, 9, 61.	2.4	2
3	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
4	Constrained iterative Hirshfeld charges: A variational approach. Journal of Chemical Physics, 2022, 156, .	1.2	2
5	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
6	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
7	ParAMS: Parameter Optimization for Atomistic and Molecular Simulations. Journal of Chemical Information and Modeling, 2021, 61, 3737-3743.	2.5	9
8	Structure-aided optimization of non-nucleoside M.Âtuberculosis thymidylate kinase inhibitors. European Journal of Medicinal Chemistry, 2021, 225, 113784.	2.6	4
9	<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
10	Reparameterization ofÂComputational Chemistry Force Fields Using GloMPO (Globally Managed) Tj ETQq0 0 0 rgBT /Overlock 10 Tf 50	1.0	0
11	Improving the Silicon Interactions of GFN-xTB. Journal of Chemical Information and Modeling, 2021, 61, 5931-5937.	2.5	5
12	Cationâ^Ï€ Interactions Accelerate the Living Cationic Ring-Opening Polymerization of Unsaturated 2-Alkyl-2-oxazolines. Macromolecules, 2020, 53, 3832-3846.	2.2	4
13	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
14	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
15	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
16	Information-Theoretic Approaches to Atoms-in-Molecules: Hirshfeld Family of Partitioning Schemes. Journal of Physical Chemistry A, 2018, 122, 4219-4245.	1.1	97
17	Ab Initio Evaluation of Henry Coefficients Using Importance Sampling. Journal of Chemical Theory and Computation, 2018, 14, 6359-6369.	2.3	12
18	Multiscale partial charge estimation on graphene for neutral, doped and charged flakes. Physical Chemistry Chemical Physics, 2018, 20, 20678-20687.	1.3	2

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19	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
20	Exploring the substrate selectivity of human sEH and M. tuberculosis EHB using QM/MM. Structural Chemistry, 2017, 28, 1501-1511.	1.0	9
21	The local response of global descriptors. Theoretical Chemistry Accounts, 2017, 136, 1.	0.5	12
22	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
23	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
24	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
25	Minimal Basis Iterative Stockholder: Atoms in Molecules for Force-Field Development. Journal of Chemical Theory and Computation, 2016, 12, 3894-3912.	2.3	119
26	Is the error on first-principles volume predictions absolute or relative?. Computational Materials Science, 2016, 117, 390-396.	1.4	15
27	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
28	An explicit approach to conceptual density functional theory descriptors of arbitrary order. Chemical Physics Letters, 2016, 660, 307-312.	1.2	46
29	The ReaxFF reactive force-field: development, applications and future directions. Npj Computational Materials, 2016, 2, .	3.5	1,319
30	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
31	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
32	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
33	Can the electronegativity equalization method predict spectroscopic properties?. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2015, 136, 76-80.	2.0	13
34	Direct computation of parameters for accurate polarizable force fields. Journal of Chemical Physics, 2014, 141, 194114.	1.2	28
35	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
36	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

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37	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
38	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
39	Assessing the Accuracy of New Geminal-Based Approaches. Journal of Physical Chemistry A, 2014, 118, 9058-9068.	1.1	77
40	New Functionalized Metalâ€“Organic Frameworks MIL-47-X (X = â^'Cl, â^'Br, â^'CH₃,) Tj ETQq0 0 0 rgBT /Overlock 10 Tf 50 Adsorption Properties. Journal of Physical Chemistry C, 2013, 117, 22784-22796.	1.5	79
41	ACKS2: Atom-condensed Kohn-Sham DFT approximated to second order. Journal of Chemical Physics, 2013, 138, 074108.	1.2	84
42	Diphosphonylation of Aromatic Diazaheterocycles and Theoretical Rationalization of Product Yields. European Journal of Organic Chemistry, 2013, 2013, 1058-1067.	1.2	21
43	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
44	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
45	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
46	Assessment of Atomic Charge Models for Gas-Phase Computations on Polypeptides. Journal of Chemical Theory and Computation, 2012, 8, 661-676.	2.3	66
47	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
48	The conformational sensitivity of iterative stockholder partitioning schemes. Chemical Physics Letters, 2012, 545, 138-143.	1.2	35
49	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
50	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
51	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
52	The Significance of Parameters in Charge Equilibration Models. Journal of Chemical Theory and Computation, 2011, 7, 1750-1764.	2.3	42
53	TAMkin: A Versatile Package for Vibrational Analysis and Chemical Kinetics. Journal of Chemical Information and Modeling, 2010, 50, 1736-1750.	2.5	155
54	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

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55	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
56	Conformational Sampling of Macrocyclic Alkenes Using a Kennardâ^'Stone-Based Algorithm. Journal of Physical Chemistry A, 2010, 114, 6879-6887.	1.1	17
57	Insight into the Solvation and Isomerization of 3â€Haloâ€1â€pazaallylic Anions from Ab Initio Metadynamics Calculations and NMR Experiments. Chemistry - A European Journal, 2009, 15, 580-584.	1.7	10
58	Multi-level Modeling of Silicaâ€“Template Interactions During Initial Stages of Zeolite Synthesis. Topics in Catalysis, 2009, 52, 1261-1271.	1.3	31
59	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
60	Molecular dynamics study of the silicaâ€“waterâ€“SDA interactions. Physical Chemistry Chemical Physics, 2009, 11, 7605.	1.3	16
61	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
62	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
63	MFI Fingerprint: How Pentasil-Induced IR Bands Shift during Zeolite Nanogrowth. Journal of Physical Chemistry C, 2008, 112, 9186-9191.	1.5	59
64	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
65	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
66	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
67	Vibrational modes in partially optimized molecular systems. Journal of Chemical Physics, 2007, 126, 224102.	1.2	95
68	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
69	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