

# Geoffrey P F Wood

## List of Publications by Year in descending order

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30  
papers

872  
citations

623574

14  
h-index

477173

29  
g-index

30  
all docs

30  
docs citations

30  
times ranked

1067  
citing authors

#	ARTICLE	IF	CITATIONS
1	A restricted-open-shell complete-basis-set model chemistry. <i>Journal of Chemical Physics</i> , 2006, 125, 094106.	1.2	208
2	Bond Dissociation Energies and Radical Stabilization Energies: An Assessment of Contemporary Theoretical Procedures. <i>Journal of Physical Chemistry A</i> , 2007, 111, 13638-13644.	1.1	101
3	Methyl Radical Addition to CS Double Bonds: Kinetic versus Thermodynamic Preferences. <i>Journal of Physical Chemistry A</i> , 2002, 106, 12124-12138.	1.1	82
4	Bond Dissociation Energies and Radical Stabilization Energies Associated with Model Peptide-Backbone Radicals. <i>Journal of Physical Chemistry A</i> , 2005, 109, 6318-6325.	1.1	72
5	Hydrogen Bond Hierarchy: Persistent Phenol- $\text{Cl}^-$ Hydrogen Bonds in the Presence of Carboxylic Acid Moieties. <i>Crystal Growth and Design</i> , 2015, 15, 4341-4354.	1.4	49
6	Harnessing Cloud Architecture for Crystal Structure Prediction Calculations. <i>Crystal Growth and Design</i> , 2018, 18, 6891-6900.	1.4	41
7	Performance of the RB3-LYP, RMP2, and UCCSD(T) Procedures in Calculating Radical Stabilization Energies for $\text{C}^{\bullet}\text{NHX}$ Radicals. <i>Journal of Physical Chemistry A</i> , 2003, 107, 7985-7990.	1.1	37
8	Templated Nucleation of Acetaminophen on Spherical Excipient Agglomerates. <i>Langmuir</i> , 2013, 29, 3292-3300.	1.6	30
9	Assessment of machine learning approaches for predicting the crystallization propensity of active pharmaceutical ingredients. <i>CrystEngComm</i> , 2019, 21, 1215-1223.	1.3	28
10	Prediction of the Relative Free Energies of Drug Polymorphs above Zero Kelvin. <i>Crystal Growth and Design</i> , 2020, 20, 5211-5224.	1.4	26
11	Nature of Glycine and Its $\dot{\text{C}}$ -Carbon Radical in Aqueous Solution: A Theoretical Investigation. <i>Journal of Chemical Theory and Computation</i> , 2008, 4, 1788-1794.	2.3	24
12	Effect of Side Chains on Competing Pathways for $\dot{\text{C}}$ -Scission Reactions of Peptide-Backbone Alkoxy Radicals. <i>Journal of Physical Chemistry A</i> , 2006, 110, 10316-10323.	1.1	19
13	Hydrogen Abstraction by Chlorine Atom from Small Organic Molecules Containing Amino Acid Functionalities: An Assessment of Theoretical Procedures. <i>Journal of Physical Chemistry A</i> , 2009, 113, 11817-11832.	1.1	18
14	Modelling nucleation from solution with the string method in the osmotic ensemble. <i>Molecular Physics</i> , 2018, 116, 2998-3007.	0.8	16
15	Drug-Excipient Interactions in the Solid State: The Role of Different Stress Factors. <i>Molecular Pharmaceutics</i> , 2017, 14, 4560-4571.	2.3	15
16	Secondary Structure Assignment of Amyloid- $\beta$ Peptide Using Chemical Shifts. <i>Journal of Chemical Theory and Computation</i> , 2011, 7, 1552-1563.	2.3	14
17	Quantitative Solution Measurement for the Selection of Complexing Agents to Enable Purification by Impurity Complexation. <i>Crystal Growth and Design</i> , 2014, 14, 3649-3657.	1.4	13
18	Dynamics and Thermodynamics of Ibuprofen Conformational Isomerism at the Crystal/Solution Interface. <i>Journal of Chemical Theory and Computation</i> , 2018, 14, 6484-6494.	2.3	13

#	ARTICLE	IF	CITATIONS
19	Kinetic Modeling of API Oxidation: (1) The AIBN/H <sub>2</sub> O/CH <sub>3</sub> OH Radical "Soup": Molecular Pharmaceutics, 2021, 18, 3037-3049.	2.3	12
20	Understanding Polymorph Selection of Sulfamerazine in Solution. Crystal Growth and Design, 2019, 19, 6925-6934.	1.4	8
21	Reactions of Benzene and 3-Methylpyrrole with the •OH and •OOH Radicals: An Assessment of Contemporary Density Functional Theory Methods. Journal of Physical Chemistry A, 2014, 118, 2667-2682.	1.1	7
22	Modeling $\hat{\gamma}^2$ -Scission Reactions of Peptide Backbone Alkoxy Radicals: A Backbone C-C Bond Fission. Journal of Chemical Theory and Computation, 2005, 1, 889-899.	2.3	6
23	Mechanistic Insights into Radical-Mediated Oxidation of Tryptophan from ab Initio Quantum Chemistry Calculations and QM/MM Molecular Dynamics Simulations. Journal of Physical Chemistry A, 2016, 120, 2926-2939.	1.1	6
24	Molecular Investigation of the Mechanism of Non-Enzymatic Hydrolysis of Proteins and the Predictive Algorithm for Susceptibility. Biochemistry, 2016, 55, 3315-3328.	1.2	6
25	Kinetic Modeling of API Oxidation: (2) Imipramine Stress Testing. Molecular Pharmaceutics, 2022, 19, 1526-1539.	2.3	6
26	Solvent Dynamics and Thermodynamics at the Crystal-Solution Interface of Ibuprofen. Crystal Growth and Design, 2019, 19, 6534-6541.	1.4	5
27	Five Degrees of Separation: Characterization and Temperature Stability Profiles for the Polymorphs of PD-0118057 (Molecule XXIII). Crystal Growth and Design, 2021, 21, 4435-4444.	1.4	4
28	Solvation of the Glycyl Radical. Journal of Physical Chemistry A, 2018, 122, 7212-7217.	1.1	3
29	Identifying Conformational Isomers of Organic Molecules in Solution via Unsupervised Clustering. Journal of Chemical Information and Modeling, 2021, 61, 2263-2273.	2.5	3
30	Investigating the Role of Solvent in the Formation of Vacancies on Ibuprofen Crystal Facets. Crystal Growth and Design, 2022, 22, 3034-3041.	1.4	0