

# Martin McCullagh

## List of Publications by Year in descending order

Source: <https://exaly.com/author-pdf/6512648/publications.pdf>

Version: 2024-02-01

40  
papers

849  
citations

567281

15  
h-index

501196

28  
g-index

49  
all docs

49  
docs citations

49  
times ranked

1169  
citing authors

#	ARTICLE	IF	CITATIONS
1	The Theory of Ultra-Coarse-Graining. 1. General Principles. Journal of Chemical Theory and Computation, 2013, 9, 2466-2480.	5.3	149
2	Modeling Self-Assembly Processes Driven by Nonbonded Interactions in Soft Materials. Journal of Physical Chemistry B, 2008, 112, 10388-10398.	2.6	78
3	Unraveling the Mystery of ATP Hydrolysis in Actin Filaments. Journal of the American Chemical Society, 2014, 136, 13053-13058.	13.7	74
4	Conformational Control of TT Dimerization in DNA Conjugates. A Molecular Dynamics Study. Journal of Physical Chemistry B, 2010, 114, 5215-5221.	2.6	62
5	DNA-Based Optomechanical Molecular Motor. Journal of the American Chemical Society, 2011, 133, 3452-3459.	13.7	56
6	Electron Donor–Acceptor Interactions with Flanking Purines Influence the Efficiency of Thymine Photodimerization. Journal of the American Chemical Society, 2011, 133, 20793-20798.	13.7	47
7	Allostery in the dengue virus NS3 helicase: Insights into the NTPase cycle from molecular simulations. PLoS Computational Biology, 2018, 14, e1006103.	3.2	38
8	Unraveling the Role of the Protein Environment for [FeFe]-Hydrogenase: A New Application of Coarse-Graining. Journal of Physical Chemistry B, 2013, 117, 4062-4071.	2.6	37
9	Conformational Control of Thymine Photodimerization in Single-Strand and Duplex DNA Containing Locked Nucleic Acid TT Steps. Journal of the American Chemical Society, 2010, 132, 12856-12858.	13.7	28
10	Conformational Control of Thymine Photodimerization in Purine-Containing Trinucleotides. Journal of Physical Chemistry Letters, 2011, 2, 1432-1438.	4.6	26
11	Electrostatic Interactions between the Bni1p Formin FH2 Domain and Actin Influence Actin Filament Nucleation. Structure, 2015, 23, 68-79.	3.3	24
12	Residue-Level Allostery Propagates through the Effective Coarse-Grained Hessian. Journal of Chemical Theory and Computation, 2020, 16, 3385-3395.	5.3	21
13	Ground and excited state electronic spectra of perylenediimide dimers with flexible and rigid geometries in DNA conjugates. Chemical Science, 2014, 5, 973-981.	7.4	19
14	Motif V regulates energy transduction between the flavivirus NS3 ATPase and RNA-binding cleft. Journal of Biological Chemistry, 2020, 295, 1551-1564.	3.4	18
15	Size-and-Shape Space Gaussian Mixture Models for Structural Clustering of Molecular Dynamics Trajectories. Journal of Chemical Theory and Computation, 2022, 18, 3218-3230.	5.3	18
16	Effect of Loop Distortion on the Stability and Structural Dynamics of DNA Hairpin and Dumbbell Conjugates. Journal of Physical Chemistry B, 2008, 112, 11415-11421.	2.6	17
17	Deterring Effect of Resins on the Aggregation of Asphaltenes in <i>n</i> -Heptane. Energy & Fuels, 2020, 34, 16081-16088.	5.1	15
18	Self-Assembly of Perylenediimide–Single-Strand–DNA Conjugates: Employing Hydrophobic Interactions and DNA Base–Base Pairing To Create a Diverse Structural Space. Chemistry - A European Journal, 2017, 23, 10328-10337.	3.3	12

#	ARTICLE	IF	CITATIONS
19	Conserved motifs in the flavivirus <sc>NS3 RNA</sc> helicase enzyme. Wiley Interdisciplinary Reviews RNA, 2022, 13, e1688.	6.4	12
20	Defects in DNA: Lessons from Molecular Motor Design. Journal of Physical Chemistry Letters, 2012, 3, 689-693.	4.6	11
21	Thymine photodimer formation in DNA hairpins. Unusual conformations favor (6 $\hat{a}$ 4) vs. (2 + 2) adducts. Photochemical and Photobiological Sciences, 2014, 13, 266-271.	2.9	10
22	Elucidating Structural Evolution of Perylene Diimide Aggregates Using Vibrational Spectroscopy and Molecular Dynamics Simulations. Journal of Physical Chemistry B, 2018, 122, 4891-4900.	2.6	10
23	Role of ATP in the RNA Translocation Mechanism of SARS-CoV-2 NSP13 Helicase. Journal of Physical Chemistry B, 2021, 125, 8787-8796.	2.6	8
24	Initial Aggregation and Ordering Mechanism of Diphenylalanine from Microsecond All-Atom Molecular Dynamics Simulations. Journal of Physical Chemistry B, 2018, 122, 12331-12341.	2.6	7
25	Electronic Interactions in Helical Stacked Arrays of the Modified DNA Base Pyrrolocytosine. Journal of Physical Chemistry B, 2012, 116, 5199-5204.	2.6	6
26	Implicit Solvation Using the Superposition Approximation (IS-SPA): An Implicit Treatment of the Nonpolar Component to Solvation for Simulating Molecular Aggregation. Journal of Chemical Theory and Computation, 2017, 13, 5911-5924.	5.3	6
27	Deriving Coarse-Grained Charges from All-Atom Systems: An Analytic Solution. Journal of Chemical Theory and Computation, 2016, 12, 4390-4399.	5.3	5
28	Characterization of the Search Complex and Recognition Mechanism of the AlkD DNA Glycosylase. Journal of Physical Chemistry B, 2019, 123, 95-105.	2.6	5
29	Molecular Dynamics Simulations of 2-Aminopurine-Labeled Dinucleoside Monophosphates Reveal Multiscale Stacking Kinetics. Journal of Physical Chemistry B, 2019, 123, 2291-2304.	2.6	4
30	The Role of Hydrophobicity in the Stability and pH-Switchability of (RXDX) <sub>4</sub> and Coumarin (RXDX) <sub>4</sub> Conjugate $\beta$ -Sheets. Journal of Physical Chemistry B, 2020, 124, 1723-1732.	2.6	3
31	RNA-Dependent Structures of the RNA-Binding Loop in the Flavivirus NS3 Helicase. Journal of Physical Chemistry B, 2020, 124, 2371-2381.	2.6	3
32	Implicit Solvation Using the Superposition Approximation (IS-SPA): Extension to Peptides in a Polar Solvent. Journal of Chemical Theory and Computation, 2021, 17, 703-713.	5.3	3
33	Modeling Catalysis in Allosteric Enzymes: Capturing Conformational Consequences. Topics in Catalysis, 0, , 1.	2.8	3
34	A Hyperactive Kunjin Virus NS3 Helicase Mutant Demonstrates Increased Dissemination and Mortality in Mosquitoes. Journal of Virology, 2020, 94, .	3.4	2
35	Theoretical Studies of Thymine Thymine Photodimerization: Using Ground State Dynamics to Model Photoreaction. , 2011, , 385-413.		1
36	Using molecular simulations to investigate how intermolecular interactions dictate liquid structure. , 2021, , 71-91.		1

#	ARTICLE	IF	CITATIONS
37	Molecular Allostery in Dengue NS3 Helicase along the ATP Hydrolysis Cycle. Biophysical Journal, 2017, 112, 497a.	0.5	0
38	Molecular Analysis of Dengue NS3 Helicase Function. Biophysical Journal, 2018, 114, 233a.	0.5	0
39	Molecular Analysis of Dengue NS3 Helicase Function. Biophysical Journal, 2019, 116, 489a-490a.	0.5	0
40	Î²-Sheet Conformations of the Flaviviridae NS3h Protein. Biophysical Journal, 2019, 116, 434a.	0.5	0