

Tetiana A Zubatiuk

List of Publications by Year in descending order

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Version: 2024-02-01

14
papers

417
citations

1163117

8
h-index

1125743

13
g-index

14
all docs

14
docs citations

14
times ranked

445
citing authors

#	ARTICLE	IF	CITATIONS
1	Development of Multimodal Machine Learning Potentials: Toward a Physics-Aware Artificial Intelligence. <i>Accounts of Chemical Research</i> , 2021, 54, 1575-1585.	15.6	78
2	Machine learned H ^{1/4} ckel theory: Interfacing physics and deep neural networks. <i>Journal of Chemical Physics</i> , 2021, 154, 244108.	3.0	25
3	Effect of Microenvironment on the Geometrical Structure of d(A) ₅ d(T) ₅ and d(G) ₅ d(C) ₅ DNA Mini-Helices and the Dickerson Dodecamer: A Density Functional Theory Study. <i>Journal of Physical Chemistry B</i> , 2020, 124, 9343-9353.	2.6	5
4	How water affects mercury-halogen interaction in the atmosphere. <i>Journal of Molecular Modeling</i> , 2019, 25, 357.	1.8	1
5	Chemical activation of biochar for energy and environmental applications: a comprehensive review. <i>Reviews in Chemical Engineering</i> , 2019, 35, 777-815.	4.4	146
6	Ultrasound cavitation intensified amine functionalization: A feasible strategy for enhancing CO ₂ capture capacity of biochar. <i>Fuel</i> , 2018, 225, 287-298.	6.4	82
7	Insight into mechanism of iron-oxides reduction in atmospheres of CH ₄ and CO. <i>Chemical Physics Letters</i> , 2018, 706, 708-714.	2.6	8
8	Modeling radical edge-site reactions of biochar in CO ₂ /water solution under ultrasonic treatment. <i>Chemical Physics Letters</i> , 2017, 689, 48-55.	2.6	2
9	Structure and Binding Energy of Double-Stranded A-DNA Mini-helices: Quantum-Chemical Study. <i>Journal of Physical Chemistry B</i> , 2015, 119, 12741-12749.	2.6	10
10	Structural Waters in the Minor and Major Grooves of DNA—A Major Factor Governing Structural Adjustments of the A-T Mini-Helix. <i>Journal of Physical Chemistry B</i> , 2015, 119, 381-391.	2.6	7
11	Molecular Structures, Relative Stability, and Proton Affinities of Nucleotides: Broad View and Novel Findings. <i>Challenges and Advances in Computational Chemistry and Physics</i> , 2014, , 137-180.	0.6	0
12	B-DNA characteristics are preserved in double stranded d(A) ₃ -d(T) ₃ and d(G) ₃ -d(C) ₃ mini-helices: conclusions from DFT/M06-2X study. <i>Physical Chemistry Chemical Physics</i> , 2013, 15, 18155.	2.8	36
13	A calculation of spectroscopic parameters for hydrogen fluoride with multi-reference state-specific coupled-cluster method. <i>Chemical Physics Letters</i> , 2010, 493, 173-178.	2.6	10
14	Dipole polarizabilities and hyperpolarizabilities of the small conjugated systems in the $\tilde{\epsilon}$ -electron coupled cluster theory. <i>Molecular Physics</i> , 2009, 107, 1729-1737.	1.7	7