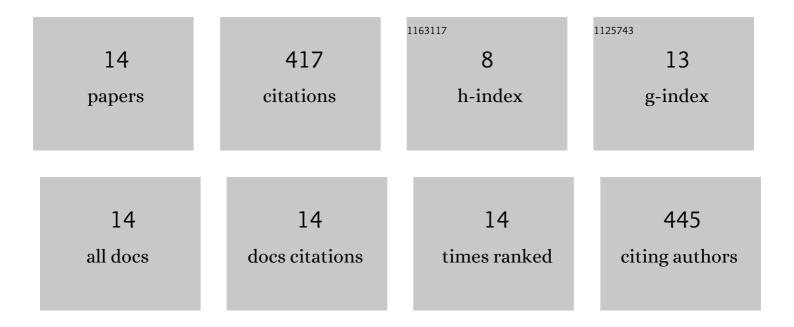
Tetiana A Zubatiuk

List of Publications by Year in descending order

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TETIANA & ZUBATULK

#	Article	IF	CITATIONS
1	Chemical activation of biochar for energy and environmental applications: a comprehensive review. Reviews in Chemical Engineering, 2019, 35, 777-815.	4.4	146
2	Ultrasound cavitation intensified amine functionalization: A feasible strategy for enhancing CO2 capture capacity of biochar. Fuel, 2018, 225, 287-298.	6.4	82
3	Development of Multimodal Machine Learning Potentials: Toward a Physics-Aware Artificial Intelligence. Accounts of Chemical Research, 2021, 54, 1575-1585.	15.6	78
4	B-DNA characteristics are preserved in double stranded d(A)3·d(T)3 and d(G)3·d(C)3 mini-helixes: conclusions from DFT/M06-2X study. Physical Chemistry Chemical Physics, 2013, 15, 18155.	2.8	36
5	Machine learned Hückel theory: Interfacing physics and deep neural networks. Journal of Chemical Physics, 2021, 154, 244108.	3.0	25
6	A calculation of spectroscopic parameters for hydrogen fluoride with multi-reference state-specific coupled-cluster method. Chemical Physics Letters, 2010, 493, 173-178.	2.6	10
7	Structure and Binding Energy of Double-Stranded A-DNA Mini-helices: Quantum-Chemical Study. Journal of Physical Chemistry B, 2015, 119, 12741-12749.	2.6	10
8	Insight into mechanism of iron-oxides reduction in atmospheres of CH4 and CO. Chemical Physics Letters, 2018, 706, 708-714.	2.6	8
9	Dipole polarizabilities and hyperpolarizabilities of the small conjugated systems in the π-electron coupled cluster theory. Molecular Physics, 2009, 107, 1729-1737.	1.7	7
10	Structural Waters in the Minor and Major Grooves of DNA—A Major Factor Governing Structural Adjustments of the A–T Mini-Helix. Journal of Physical Chemistry B, 2015, 119, 381-391.	2.6	7
11	Effect of Microenvironment on the Geometrical Structure of d(A) ₅ d(T) ₅ and d(G) ₅ d(C) ₅ DNA Mini-Helixes and the Dickerson Dodecamer: A Density Functional Theory Study. Journal of Physical Chemistry B, 2020, 124, 9343-9353.	2.6	5
12	Modeling radical edge-site reactions of biochar in CO2/water solution under ultrasonic treatment. Chemical Physics Letters, 2017, 689, 48-55.	2.6	2
13	How water affects mercury–halogen interaction in the atmosphere. Journal of Molecular Modeling, 2019, 25, 357.	1.8	1
14	Molecular Structures, Relative Stability, and Proton Affinities of Nucleotides: Broad View and Novel Findings. Challenges and Advances in Computational Chemistry and Physics, 2014, , 137-180.	0.6	0