

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 | 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 |
| 2 | 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 |
| 3 | 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 |
| 4 | 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/MO6-2X study. <i>Physical Chemistry Chemical Physics</i> , 2013, 15, 18155. | 2.8 | 36 |
| 5 | Machine learned H ₂ molecule theory: Interfacing physics and deep neural networks. <i>Journal of Chemical Physics</i> , 2021, 154, 244108. | 3.0 | 25 |
| 6 | 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 |
| 7 | 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 |
| 8 | 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 |
| 9 | Dipole polarizabilities and hyperpolarizabilities of the small conjugated systems in the ĩ€-electron coupled cluster theory. <i>Molecular Physics</i> , 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. <i>Journal of Physical Chemistry B</i> , 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-Helices and the Dickerson Dodecamer: A Density Functional Theory Study. <i>Journal of Physical Chemistry B</i> , 2020, 124, 9343-9353. | 2.6 | 5 |
| 12 | 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 |
| 13 | How water affects mercury-halogen interaction in the atmosphere. <i>Journal of Molecular Modeling</i> , 2019, 25, 357. | 1.8 | 1 |
| 14 | 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 |