

Bardi Benediktsson

List of Publications by Year in descending order

Source: <https://exaly.com/author-pdf/3151430/publications.pdf>

Version: 2024-02-01

5
papers

214
citations

1684188

5
h-index

2053705

5
g-index

5
all docs

5
docs citations

5
times ranked

150
citing authors

#	ARTICLE	IF	CITATIONS
1	QM/MM Study of the Nitrogenase MoFe Protein Resting State: Broken-Symmetry States, Protonation States, and QM Region Convergence in the FeMoco Active Site. <i>Inorganic Chemistry</i> , 2017, 56, 13417-13429.	4.0	74
2	QM/MM calculations reveal a bridging hydroxo group in a vanadium nitrogenase crystal structure. <i>Chemical Communications</i> , 2018, 54, 7310-7313.	4.1	51
3	A model for dinitrogen binding in the E ₄ state of nitrogenase. <i>Chemical Science</i> , 2019, 10, 11110-11124.	7.4	48
4	Quantum Mechanics/Molecular Mechanics Study of Resting-State Vanadium Nitrogenase: Molecular and Electronic Structure of the Iron–Vanadium Cofactor. <i>Inorganic Chemistry</i> , 2020, 59, 11514-11527.	4.0	25
5	Analysis of the Geometric and Electronic Structure of Spin-Coupled Iron–Sulfur Dimers with Broken-Symmetry DFT: Implications for FeMoco. <i>Journal of Chemical Theory and Computation</i> , 2022, 18, 1437-1457.	5.3	16