

Edvin Erdtman

List of Publications by Year in descending order

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14
papers

215
citations

1163117

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1058476

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docs citations

15
times ranked

308
citing authors

#	ARTICLE	IF	CITATIONS
1	Simulation of $\hat{1}\pm$ - and $\hat{1}^2$ -PVDF melting mechanisms. <i>Polymer</i> , 2012, 53, 2919-2926.	3.8	57
2	Molecular modelling of oxygen and water permeation in polyethylene. <i>Polymer</i> , 2013, 54, 2988-2998.	3.8	27
3	Computational studies on Schiff-base formation: Implications for the catalytic mechanism of porphobilinogen synthase. <i>Computational and Theoretical Chemistry</i> , 2011, 963, 479-489.	2.5	24
4	Time evolution of the CO ₂ hydrogenation to fuels over Cu-Zr-SBA-15 catalysts. <i>Journal of Catalysis</i> , 2018, 362, 55-64.	6.2	19
5	Modelling the behavior of 5-aminolevulinic acid and its alkyl esters in a lipid bilayer. <i>Chemical Physics Letters</i> , 2008, 463, 178-182.	2.6	17
6	Computational Insights into the Mechanism of Porphobilinogen Synthase. <i>Journal of Physical Chemistry B</i> , 2010, 114, 16860-16870.	2.6	17
7	The first branching point in porphyrin biosynthesis: A systematic docking, molecular dynamics and quantum mechanical/molecular mechanical study of substrate binding and mechanism of uroporphyrinogenâ€”III decarboxylase. <i>Journal of Computational Chemistry</i> , 2011, 32, 822-834.	3.3	17
8	A molecular-level computational study of the diffusion and solubility of water and oxygen in carbonaceous polyethylene nanocomposites. <i>Journal of Polymer Science, Part B: Polymer Physics</i> , 2016, 54, 589-602.	2.1	10
9	Matching precursor kinetics to afford a more robust CVD chemistry: a case study of the C chemistry for silicon carbide using SiF ₄ as Si precursor. <i>Journal of Materials Chemistry C</i> , 2017, 5, 5818-5823.	5.5	7
10	Catalytic Mechanism of Porphobilinogen Synthase: The Chemical Step Revisited by QM/MM Calculations. <i>Journal of Physical Chemistry B</i> , 2012, 116, 12105-12112.	2.6	6
11	Theoretical study of 5-aminolevulinic acid (5ALA) and some pharmaceutically important derivatives. <i>Chemical Physics Letters</i> , 2007, 434, 101-106.	2.6	4
12	Simulations of the thermodynamics and kinetics of NH ₃ at the RuO ₂ (110) surface. <i>Surface Science</i> , 2017, 656, 77-85.	1.9	4
13	Theoretical Study of 5-Aminolevulinic Acid Tautomerization:â€” A Novel Self-Catalyzed Mechanism. <i>Journal of Physical Chemistry A</i> , 2008, 112, 4367-4374.	2.5	2
14	Permeability of 5-aminolevulinic acid oxime derivatives in lipid membranes. <i>Theoretical Chemistry Accounts</i> , 2016, 135, 1.	1.4	0