Wim Buijs

List of Publications by Year in descending order

19 papers	293 citations	840776 11 h-index	888059 17 g-index
19 all docs	19 docs citations	19 times ranked	448 citing authors

#	Article	IF	Citations
1	Atomistic understanding of cation exchange in PbS nanocrystals using simulations with pseudoligands. Nature Communications, 2016, 7, 11503.	12.8	48
2	Solubility of sulfur compounds in commercial physical solvents and an ionic liquid from Monte Carlo simulations. Fluid Phase Equilibria, 2017, 433, 50-55.	2.5	29
3	Correlation between Quantumchemically Calculated LUMO Energies and the Electrochemical Window of Ionic Liquids with Reduction-Resistant Anions. International Journal of Electrochemistry, 2012, 2012, 1-6.	2.4	27
4	Direct Air Capture of CO₂ with an Amine Resin: A Molecular Modeling Study of the CO₂ Capturing Process. Industrial & Engineering Chemistry Research, 2017, 56, 12297-12304.	3.7	27
5	Molecular Modeling Study toward Development of H₂S-Free Removal of Iron Sulfide Scale from Oil and Gas Wells. Industrial & Engineering Chemistry Research, 2018, 57, 10095-10104.	3.7	24
6	Shape-selective diisopropylation of naphthalene in H-Mordenite: Myth or reality?. Journal of Catalysis, 2010, 270, 60-66.	6.2	16
7	Catalytic and molecular separation properties of Zeogrids and Zeotiles. Catalysis Today, 2011, 168, 17-27.	4.4	15
8	Thermodynamic and Transport Properties of Crown-Ethers: Force Field Development and Molecular Simulations. Journal of Physical Chemistry B, 2017, 121, 8367-8376.	2.6	15
9	Molecular structure of dextran sulphate sodium in aqueous environment. Journal of Molecular Structure, 2018, 1156, 320-329.	3.6	14
10	Crystal structure, stability, and electronic properties of hydrated metal sulfates MSO4(H2O)n (M=Ni,) Tj ETQq0 0 0 rgBT /Overlock 10 Tf 77-86.	3.8	13
11	Direct Air Capture of CO₂ with an Amine Resin: A Molecular Modeling Study of the Oxidative Deactivation Mechanism with O₂. Industrial & Engineering Chemistry Research, 2019, 58, 17760-17767.	3.7	13
12	Separation of diisopropylnaphthalene isomers. Journal of Chromatography A, 2009, 1216, 6410-6416.	3.7	11
13	Shape-selective synthesis of 2,6-diisopropylnaphthalene on H-mordenite catalysts. Journal of Catalysis, 2012, 292, 181-187.	6.2	10
14	Direct Air Capture of CO₂ with an Amine Resin: A Molecular Modeling Study of the Deactivation Mechanism by CO₂. Industrial & Engineering Chemistry Research, 2019, 58, 14705-14708.	3.7	10
15	Molecular Modeling Study to the Relation between Structure of LPEI, Including Water-Induced Phase Transitions and CO₂ Capturing Reactions. Industrial & Engineering Chemistry Research, 2021, 60, 11309-11316.	3.7	8
16	CO2 solubility in small carboxylic acids: Monte Carlo simulations and PC-SAFT modeling. Fluid Phase Equilibria, 2018, 458, 1-8.	2.5	7
17	Molecular Modeling Study of the SO₂ Deactivation of an Amine Resin and a Procedure To Avoid SO₂ Deactivation Using a Polyethylene Glycol/Tertiary Amine System. Industrial & Engineering Chemistry Research, 2020, 59, 13388-13395.	3.7	3
18	Reply to the letter of Robert Brzozowski concerning the conclusions drawn in â€œShape-selective diisopropylation of naphthalene in H-Mordenite: Myth or reality?â€• Journal of Catalysis, 2011, 280, 142-143.	6.2	2

#	Article	IF	Citations
19	Reply to the â€œComments on Shape-selective diisopropylation of naphthalene in H-mordenite: Myth or reality?â€•by Gyula Tasi and IstvÃ¡n PÃ¡linkÃ³. Journal of Catalysis, 2011, 279, 231.	6.2	1