Jeroen Van der Mynsbrugge

List of Publications by Year
in descending order

24	1,747	394421 19	580821 25
papers	citations	h-index	g-index

29	29	29	1377
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Unraveling the Reaction Mechanisms Governing Methanolâ€toâ€Olefins Catalysis by Theory and Experiment. ChemPhysChem, 2013, 14, 1526-1545.	2.1	232
2	First principle chemical kinetics in zeolites: the methanol-to-olefin process as a case study. Chemical Society Reviews, 2014, 43, 7326-7357.	38.1	188
3	First Principle Kinetic Studies of Zeolite-Catalyzed Methylation Reactions. Journal of the American Chemical Society, 2011, 133, 888-899.	13.7	153
4	Methylation of benzene by methanol: Single-site kinetics over H-ZSM-5 and H-beta zeolite catalysts. Journal of Catalysis, 2012, 292, 201-212.	6.2	126
5	Full Theoretical Cycle for both Ethene and Propene Formation during Methanolâ€toâ€Olefin Conversion in Hâ€ZSMâ€5. ChemCatChem, 2011, 3, 208-212.	3.7	116
6	Effect of temperature and branching on the nature and stability of alkene cracking intermediates in H-ZSM-5. Journal of Catalysis, 2017, 345, 53-69.	6.2	92
7	Molecular Dynamics Kinetic Study on the Zeolite-Catalyzed Benzene Methylation in ZSM-5. ACS Catalysis, 2013, 3, 2556-2567.	11.2	91
8	Assembly of cyclic hydrocarbons from ethene and propene in acid zeolite catalysis to produce active catalytic sites for MTO conversion. Journal of Catalysis, 2010, 271, 67-78.	6.2	86
9	Characterization of Isolated Ga³⁺ Cations in Ga/H-MFI Prepared by Vapor-Phase Exchange of H-MFI Zeolite with GaCl₃. ACS Catalysis, 2018, 8, 6106-6126.	11.2	85
10	Efficient Approach for the Computational Study of Alcohol and Nitrile Adsorption in H-ZSM-5. Journal of Physical Chemistry C, 2012, 116, 5499-5508.	3.1	77
11	Mechanistic Studies on Chabaziteâ€Type Methanolâ€toâ€Olefin Catalysts: Insights from Timeâ€Resolved UV/Vis Microspectroscopy Combined with Theoretical Simulations. ChemCatChem, 2013, 5, 173-184.	3.7	70
12	How Chain Length and Branching Influence the Alkene Cracking Reactivity on H-ZSM-5. ACS Catalysis, 2018, 8, 9579-9595.	11.2	70
13	Insight into the Formation and Reactivity of Frameworkâ€Bound Methoxide Species in Hâ€ZSMâ€5 from Static and Dynamic Molecular Simulations. ChemCatChem, 2014, 6, 1906-1918.	3.7	69
14	Enthalpy and Entropy Barriers Explain the Effects of Topology on the Kinetics of Zeoliteâ€Catalyzed Reactions. Chemistry - A European Journal, 2013, 19, 11568-11576.	3.3	63
15	On the stability and nature of adsorbed pentene in BrÃ¸nsted acid zeolite H-ZSM-5 at 323 K. Journal of Catalysis, 2016, 340, 227-235.	6.2	55
16	Theoretical Analysis of the Influence of Pore Geometry on Monomolecular Cracking and Dehydrogenation ofn-Butane in BrÃ¸nsted Acidic Zeolites. ACS Catalysis, 2017, 7, 2685-2697.	11.2	42
17	Impact of long-range electrostatic and dispersive interactions on theoretical predictions of adsorption and catalysis in zeolites. Catalysis Today, 2018, 312, 51-65.	4.4	35
18	Facing the Challenges of Borderline Oxidation State Assignments Using State-of-the-Art Computational Methods. Inorganic Chemistry, 2020, 59, 15410-15420.	4.0	27

#	Article	IF	Citations
19	Understanding BrÃ¸nstedâ€Acid Catalyzed Monomolecular Reactions of Alkanes in Zeolite Pores by Combining Insights from Experiment and Theory. ChemPhysChem, 2018, 19, 341-358.	2.1	21
20	Computational modeling predicts the stability of both Pd⁺ and Pd²⁺ ion-exchanged into H-CHA. Journal of Materials Chemistry A, 2021, 9, 2161-2174.	10.3	20
21	Investigation of the modes of NO adsorption in Pd/H-CHA. Applied Catalysis B: Environmental, 2022, 304, 120992.	20.2	18
22	Challenges for the theoretical description of the mechanism and kinetics of reactions catalyzed by zeolites. Journal of Catalysis, 2021, 404, 832-849.	6.2	6
23	Response to â€œImpact of Zeolite Structure on Entropicâ€“Enthalpic Contributions to Alkane Monomolecular Cracking: An IR Operando Studyâ€• Chemistry - A European Journal, 2019, 25, 7225-7226.	3.3	1
24	Understanding BrÃ¸nsted-Acid Catalyzed Monomolecular Reactions of Alkanes in Zeolite Pores by Combining Insights from Experiment and Theory. ChemPhysChem, 2018, 19, 338-338.	2.1	0