

# Kristof De Wispelaere

## List of Publications by Year in descending order

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29  
papers

2,347  
citations

201674

27  
h-index

454955

30  
g-index

33  
all docs

33  
docs citations

33  
times ranked

1813  
citing authors

#	ARTICLE	IF	CITATIONS
1	Mechanistic Insight into the Framework Methylation of H-ZSM-5 for Varying Methanol Loadings and Si/Al Ratios Using First-Principles Molecular Dynamics Simulations. ACS Catalysis, 2020, 10, 8904-8915.	11.2	36
2	Insight into the effects of confined hydrocarbon species on the lifetime of methanol conversion catalysts. Nature Materials, 2020, 19, 1081-1087.	27.5	52
3	A Supramolecular View on the Cooperative Role of Brønsted and Lewis Acid Sites in Zeolites for Methanol Conversion. Journal of the American Chemical Society, 2019, 141, 14823-14842.	13.7	80
4	Ethene Dimerization on Zeolite-Hosted Ni Ions: Reversible Mobilization of the Active Site. ACS Catalysis, 2019, 9, 5645-5650.	11.2	54
5	Collective action of water molecules in zeolite dealumination. Catalysis Science and Technology, 2019, 9, 3721-3725.	4.1	43
6	Effect of Zeolite Topology and Reactor Configuration on the Direct Conversion of CO <sub>2</sub> to Light Olefins and Aromatics. ACS Catalysis, 2019, 9, 6320-6334.	11.2	144
7	On the intrinsic dynamic nature of the rigid UiO-66 metal-organic framework. Chemical Science, 2018, 9, 2723-2732.	7.4	41
8	Understanding zeolite-catalyzed benzene methylation reactions by methanol and dimethyl ether at operating conditions from first principle microkinetic modeling and experiments. Catalysis Today, 2018, 312, 35-43.	4.4	28
9	How Chain Length and Branching Influence the Alkene Cracking Reactivity on H-ZSM-5. ACS Catalysis, 2018, 8, 9579-9595.	11.2	70
10	Structure-performance descriptors and the role of Lewis acidity in the methanol-to-propylene process. Nature Chemistry, 2018, 10, 804-812.	13.6	221
11	Entropy Contributions to Transition State Modeling. , 2018, , 189-228.		5
12	Benzene co-reaction with methanol and dimethyl ether over zeolite and zeotype catalysts: Evidence of parallel reaction paths to toluene and diphenylmethane. Journal of Catalysis, 2017, 349, 136-148.	6.2	70
13	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
14	Hydrogen Transfer versus Methylation: On the Genesis of Aromatics Formation in the Methanol-To-Hydrocarbons Reaction over H-ZSM-5. ACS Catalysis, 2017, 7, 5773-5780.	11.2	102
15	Suppression of the Aromatic Cycle in Methanol-to-Olefins Reaction over ZSM-5 by Post-Synthetic Modification Using Calcium. ChemCatChem, 2016, 8, 3057-3063.	3.7	71
16	On the stability and nature of adsorbed pentene in Brønsted acid zeolite H-ZSM-5 at 323 K. Journal of Catalysis, 2016, 340, 227-235.	6.2	55
17	Insight into the Effect of Water on the Methanol-to-Olefins Conversion in H-SAPO-34 from Molecular Simulations and in Situ Microspectroscopy. ACS Catalysis, 2016, 6, 1991-2002.	11.2	110
18	Towards molecular control of elementary reactions in zeolite catalysis by advanced molecular simulations mimicking operating conditions. Catalysis Science and Technology, 2016, 6, 2686-2705.	4.1	38

#	ARTICLE	IF	CITATIONS
19	How zeolitic acid strength and composition alter the reactivity of alkenes and aromatics towards methanol. <i>Journal of Catalysis</i> , 2015, 328, 186-196.	6.2	49
20	Complex Reaction Environments and Competing Reaction Mechanisms in Zeolite Catalysis: Insights from Advanced Molecular Dynamics. <i>Chemistry - A European Journal</i> , 2015, 21, 9385-9396.	3.3	53
21	Shape-Selective Diffusion of Olefins in 8-Ring Solid Acid Microporous Zeolites. <i>Journal of Physical Chemistry C</i> , 2015, 119, 23721-23734.	3.1	65
22	First principle chemical kinetics in zeolites: the methanol-to-olefin process as a case study. <i>Chemical Society Reviews</i> , 2014, 43, 7326-7357.	38.1	188
23	Insight into the Formation and Reactivity of Framework-Bound Methoxide Species in H-ZSM-5 from Static and Dynamic Molecular Simulations. <i>ChemCatChem</i> , 2014, 6, 1906-1918.	3.7	69
24	Molecular Dynamics Kinetic Study on the Zeolite-Catalyzed Benzene Methylation in ZSM-5. <i>ACS Catalysis</i> , 2013, 3, 2556-2567.	11.2	91
25	Mechanistic Studies on Chabazite-Type Methanol-to-Olefin Catalysts: Insights from Time-Resolved UV/Vis Microspectroscopy Combined with Theoretical Simulations. <i>ChemCatChem</i> , 2013, 5, 173-184.	3.7	70
26	Unraveling the Reaction Mechanisms Governing Methanol-to-Olefins Catalysis by Theory and Experiment. <i>ChemPhysChem</i> , 2013, 14, 1526-1545.	2.1	232
27	Complete low-barrier side-chain route for olefin formation during methanol conversion in H-SAPO-34. <i>Journal of Catalysis</i> , 2013, 305, 76-80.	6.2	102
28	Identification of Intermediates in Zeolite-Catalyzed Reactions by In Situ UV/Vis Microspectroscopy and a Complementary Set of Molecular Simulations. <i>Chemistry - A European Journal</i> , 2013, 19, 16595-16606.	3.3	68
29	Experimental and theoretical IR study of methanol and ethanol conversion over H-SAPO-34. <i>Catalysis Today</i> , 2011, 177, 12-24.	4.4	41