# Kristof De Wispelaere

List of Publications by Year
in descending order

Source: https://exaly.com/author-pdf/7730393/publications.pdf

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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 | Unraveling the Reaction Mechanisms Governing Methanolâ€toâ€Olefins Catalysis by Theory and Experiment. ChemPhysChem, 2013, 14, 1526-1545. | 2.1 | 232 |
| 2 | Structureâ€“performance descriptors and the role of Lewis acidity in the methanol-to-propylene process. Nature Chemistry, 2018, 10, 804-812. | 13.6 | 221 |
| 3 | 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 |
| 4 | 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 |
| 5 | 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 |
| 6 | Complete low-barrier side-chain route for olefin formation during methanol conversion in H-SAPO-34. Journal of Catalysis, 2013, 305, 76-80. | 6.2 | 102 |
| 7 | 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 |
| 8 | 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 |
| 9 | Molecular Dynamics Kinetic Study on the Zeolite-Catalyzed Benzene Methylation in ZSM-5. ACS Catalysis, 2013, 3, 2556-2567. | 11.2 | 91 |
| 10 | A Supramolecular View on the Cooperative Role of BrÃ¸nsted and Lewis Acid Sites in Zeolites for Methanol Conversion. Journal of the American Chemical Society, 2019, 141, 14823-14842. | 13.7 | 80 |
| 11 | Suppression of the Aromatic Cycle in Methanolâ€toâ€Olefins Reaction over ZSMâ€5 by Postâ€Synthetic Modification Using Calcium. ChemCatChem, 2016, 8, 3057-3063. | 3.7 | 71 |
| 12 | 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 |
| 13 | 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 |
| 14 | How Chain Length and Branching Influence the Alkene Cracking Reactivity on H-ZSM-5. ACS Catalysis, 2018, 8, 9579-9595. | 11.2 | 70 |
| 15 | 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 |
| 16 | Identification of Intermediates in Zeoliteâ€Catalyzed Reactions by In Situ UV/Vis Microspectroscopy and a Complementary Set of Molecular Simulations. Chemistry - A European Journal, 2013, 19, 16595-16606. | 3.3 | 68 |
| 17 | Shape-Selective Diffusion of Olefins in 8-Ring Solid Acid Microporous Zeolites. Journal of Physical Chemistry C, 2015, 119, 23721-23734. | 3.1 | 65 |
| 18 | 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 |

| # | Article | IF | Citations |
|---|---|---|---|
| 19 | Ethene Dimerization on Zeolite-Hosted Ni Ions: Reversible Mobilization of the Active Site. ACS Catalysis, 2019, 9, 5645-5650. | 11.2 | 54 |
| 20 | Complex Reaction Environments and Competing Reaction Mechanisms in Zeolite Catalysis: Insights from Advanced Molecular Dynamics. Chemistry - A European Journal, 2015, 21, 9385-9396. | 3.3 | 53 |
| 21 | Insight into the effects of confined hydrocarbon species on the lifetime of methanol conversion catalysts. Nature Materials, 2020, 19, 1081-1087. | 27.5 | 52 |
| 22 | How zeolitic acid strength and composition alter the reactivity of alkenes and aromatics towards methanol. Journal of Catalysis, 2015, 328, 186-196. | 6.2 | 49 |
| 23 | Collective action of water molecules in zeolite dealumination. Catalysis Science and Technology, 2019, 9, 3721-3725. | 4.1 | 43 |
| 24 | Experimental and theoretical IR study of methanol and ethanol conversion over H-SAPO-34. Catalysis Today, 2011, 177, 12-24. | 4.4 | 41 |
| 25 | On the intrinsic dynamic nature of the rigid UiO-66 metalâ€“organic framework. Chemical Science, 2018, 9, 2723-2732. | 7.4 | 41 |
| 26 | 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 |
| 27 | 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 |
| 28 | 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 |
| 29 | Entropy Contributions to Transition State Modeling. , 2018, , 189-228. | | 5 |