Report Tier1 project

Project name: Dynamical kinetic study of zeolite-catalyzed reactions

Users: Kristof De Wispelaere, Jeroen Van der Mynsbrugge, Sam Moors, Veronique Van Speybroeck, Karen Hemelsoet, Pieter Cnudde, Andy Van Yperen – De Deyne

Period: 07/07/2014 – 31/12/2014

Awarded nodedays: 4371

Used nodedays: 4378.5

Total price: €2539.51

Usage per user

User ID	Name	Used nodedays	Cost (€)
vsc40490	Kristof	2421.5	1404.462
vsc40585	Sam	35.7	20.72282
vsc40163	Jeroen	753.0	436.7625
vsc40056	Karen	330.8	191.8409
vsc40175	Andy	408.8	237.0783
vsc40920	Pieter	428.7	248.6403

Projects / publications the results are used for

1. The computing time of Kristof De Wispelaere (vsc40490) included molecular dynamics simulations, metadynamics simulations and TPS calculation (CP2K) on proton mobility and methoxide formation in water, methanol and water-methanol mixtures adsorbed in H-SAPO-34, benzene methylation by methanol in H-SSZ-24 and H-SAPO-5 and the adsorption of pentene and pentoxides in H-ZSM-5. The corresponding results are/will be used in the following publications:
    - "Exploring new frontiers in modeling complex zeolite-catalyzed reactions using advanced molecular dynamics techniques", K. De Wispelaere, B. Ensing, A. Ghysels, E.J. Meijer, V. Van Speybroeck, *Chem. Eur. J.*, Submitted, 2015
    - "How zeolitic acid strength and composition alter the reactivity of alkenes and aromatics towards methanol", M.Westgård Erichsen*, **K. De Wispelaere***, K. Hemelsoet, S.L.C. Moors, T. Deconinck, M. Waroquier, S. Svelle, V. Van Speybroeck, U. Olsbye, *J. Catal.*, In press, 2015 (* authors contributed equally)
    - "Influence of water on the MTO reaction in H-SAPO-34", Kristof De Wispelaere et al. in preparation

- "Surface interactions and reactivity of pentene on H-ZSM-5 – a study combining theory and experiment", S. Schallmoser, J. Van der Mynsbrugge, K. De Wispelaere, M. Waroquier, G.L. Haller, M. Sanchez-Sanchez, V. Van Speybroeck, J.A. Lercher, in preparation

2. The computing time of Sam Moors (vsc40585) was used for molecular dynamics and metadynamics simulations (CP2K) on the methylation of methyl substituted benzenes by dimethylether in H-ZSM-5. The results will be used in a publication in collaboration with researchers from the University of Oslo (Unni, Olsbye, Stian Svelle).

3. The computing time of Jeroen Van der Mynsbrugge (vsc40163) was used for molecular dynamics simulations (CP2K) on the adsorption of pentene and pentoxides in H-ZSM-5. The results are being used in "Surface interactions and reactivity of pentene on H-ZSM-5 – a study combining theory and experiment", S. Schallmoser, J. Van der Mynsbrugge, K. De Wispelaere, M. Waroquier, G.L. Haller, M. Sanchez-Sanchez, V. Van Speybroeck, J.A. Lercher, in preparation

4. The Tier1 computing time of Karen Hemelsoet (vsc40056) and Andy Van Yperen-De Deyne (vsc40175) included optimizations and ab initio MD simulations on copper-containing zeolites used as catalyst for the reduction of nitrogen oxides. The simulations are performed with the CP2K program and are used to compute IR spectra. The resulting spectra are currently analyzed and will be included in a publication in collaboration with experimental partners of University College London (Dr. A. Beale, I. Lezcano-Gonzalez).

5. Pieter Cnudde (vsc40920) performed molecular dynamics simulations in CP2K on adsorbed pentene, pentyl and octyl cations in H-ZSM-5. These simulations were performed in the framework of a collaboration with the group of J. Lercher on alkene cracking.