Report Tier1 project

Project name: High-throughput screening of ternary tungsten alloys with DFT

Users: Kurt Lejaeghere, Lennart Joos, Pieter Cnudde

Period: 04/07/2014 – 31/12/2014

Awarded node days: 4000

Used node days: 3774.5

Total price: € 2189.21

Usage per user

User ID	Name	Used node days
vsc40323	Kurt Lejaeghere	1120.1
vsc40460	Lennart Joos	850.0
vsc40920	Pieter Cnudde	1804.3

Projects / publications the results are used for

1. The computing time of Kurt Lejaeghere mainly served to wrap up the high-throughput screening of tungsten ternaries for fusion purposes. This research was part of Kurt Lejaeghere's PhD project (FWO). Whereas the previous Tier1 project "High-throughput screenen van ternaire wolfraamlegeringen met DFT" focused on 4d and 5d dopants, the present project aimed to calculate the mechanical properties, energy and band structure of W30XY cells with X and / or Y a 3d transition metal and the other dopant a 4d or 5d transition metal. In practice, not all 3d ternaries could be computed yet due to VASP errors in approximately 40 structures (out of 182). This called for a manual treatment, which took much more human input. When these remaining structures are finished, all results will be processed (i.e. analyzed in a Pareto study and screened based on ductility descriptors) and published. This publication is foreseen to be submitted near the end of the summer of 2015 (end of the manual calculations by March 2015 on Tier2 infrastructure, analysis will take additional time).
   Several smaller calculations were submitted as well, the most important ones related to a Monte Carlo study of the error properties of an equation of state. These results are currently being written down, and submittal is foreseen for March 2015.
2. The computing time of Lennart Joos was used for metadynamics simulations of the opening/closing behavior of a newly discovered zeolite, COK-14. [1,2] The size of the system and necessary simulation time were too large to run the calculations on the Ghent University computer infrastructure within a reasonable time.
   The work was performed within the Interuniversity Attraction Poles Programme (P7/05) initiated by the Belgian Science Policy Office, in close collaboration with the experimental partner (Centrum voor Oppervlaktechemie en Katalyse) in Leuven. Another publication is expected soon.
   [1] Design of zeolite by inverse sigma transformation , E. Verheyen, L. Joos, K. Van Havenbergh, N. Kasian, E. Gobechiya, K. Houthoofd, M. Hinterstein, E. Breynaerts, V. Van Speybroeck, M. Waroquier, S. Bals, G. Van Tendeloo, C. Kirschhock, J.A. Martens , Nature

Materials , 11 (12), 1059-1064, 2012 , IF: 35.749

[2] Reversible transformation of flexible periodically interrupted -COK-14 to rigid fully connected OKO zeolite , E. Verheyen, L. Joos, C. Martineau, C.J. Dawson, C. Weidenthaler, W. Schmidt, R. Yuan, E. Breynaerts, V. Van Speybroeck, M. Waroquier, F. Taulelle, M.M.J. Treacy, J.A. Martens, C. Kirschhock , Materials Horizons, Vol. 1 , 582 - 587 , 2014

3. The computing time of Pieter Cnudde mainly served to perform ab initio molecular dynamics simulations on several C_5 guest species in H-ZSM-5. To study the adsorption properties of pentene in the zeolitic environment, both pentyl cations, pentoxide species and physisorbed pentene complexes were simulated at relevant temperatures for cracking processes. Long runs of approximately 100 ps were performed in order to provide sufficiently long sampling periods to extract accurate thermodynamical properties. This set of simulations forms the basis for a further metadynamics study on the cracking reaction of pentene itself. The entire computing time can be situated in Pieter Cnudde's PhD Research: "Adsorption, oligomerization and C-C cracking of C_4-C_{10} alkenes in zeolite materials: insights from ab initio molecular dynamics simulations" and the results will be published in the course of his PhD.