Report Tier1 project

Project name: Assessing the accuracy of a screened hybrid functional for property predictions of elemental solids

Users: Kurt Lejaeghere

Period: 15/03/2015 – 15/11/2015

Awarded node days: 1742

Used node days: 1745.7

Usage per user

User ID	Name	Used node days
vsc40323	Kurt Lejaeghere	1745.7

Projects / publications the results are used for

The computing time of Kurt Lejaeghere mainly served to determine the equations of state of the ground-state elemental crystal with the HSE functional. 37 elements have been fully completed so far, 4 need to be redone with spin-orbit coupling, 20 need to be redone with more stringent computational settings and the remaining 10 have not started yet due to VASP errors. Only the last 10 cases are expected to still take a significant amount of time. This work is expected to take a few more months, and a publication is foreseen for early 2016 in collaboration with the VASP group, after a full statistical analysis of the results with respect to experiment has been performed.

Two other topics were investigated with the computing time of the present Tier1 project. Monte Carlo simulations were performed to study the error properties of an equation of state. A manuscript has been written on these results, and will be submitted in the next week. The Tier1 time was also used during a research stay in Vienna to perform convergence tests on ACFDT-RPA, an advanced electronic-structure method that allows the incorporation of more accurate electron correlation. No immediate publication is planned for these results, but the convergence test results will be used to execute an extensive benchmark of RPA for a wide range of solids. This work is planned for 2016, and may lead to a publication in 2017. Other RPA work, on specialized applications, may be performed earlier (e.g. RPA calculations for zeolites and MOFs).