Basically, we used the awarded 2304 node days for the following projects;

1. Hybrid functional calculations of aldol condensations pathways
   status: in preparation

   In this work, hybrid functional calculations on periodic models have been performed (1) to truthfully compare the periodic and cluster calculations; (2) to more accurately describe environmental effects. Due to the size of the systems and the amount of calculations that need to be performed, it is clear that these calculations go beyond what can comfortably be done (within a reasonable timeframe) on a TIER2 cluster. All calculations have finished; the obtained free energy profiles for both periodic and cluster computation compare well. The stabilization effect due to the environment is more pronounced in the description of some reaction steps predicted by periodic calculations. The paper will be submitted end December 2014. As not all computational time was granted in the previous Tier1 project, we decided to compute only a part of the intended calculations. {~ 1500 node days used}

2. Au@UiO-66: an oxidation catalyst
   status: submitted to Journal of Catalysis

   In this work, a new UiO-66 MOF with embedded gold Nanoparticles was experimentally synthesized, characterized (via N_2 sorption, XRPD, UV-Vis, XRF, XPS and TEM analysis). The Au@UiO-66 was furthermore tested in several catalytic reactions, however, the mechanism remained unclear and spectroscopic efforts (IR, Raman) in combination with molecular modelling were required to unravel possible reaction paths. We performed periodic MD-simulations (NVT/NPT) to unravel an experimentally obtained IR-spectrum. From our simulations, we constructed velocity power spectra to distinguish between adsorbed and chemisorbed pentanol species. All calculations are completed and the paper has been submitted in November 2014. {~ 800 node days used}