

Report Tier1 project:

**The electronic and magnetic structure of  
Breathing Metal-Organic Frameworks**

date

21-11-2014

## 1. General Project Information

<b>Title</b>	<i>The electronic and magnetic structure of Breathing Metal-Organic Frameworks.</i>		
<b>Applicant</b>	Dr. Dr. Danny E.P. Vanpoucke		
<b>Pomoter</b>	Prof. Dr. ir. V. Van Speybroeck		
<b>Other Users</b>	ir. Michael Sluydts		
<b>Financing</b>	First principle chemical kinetics in nanoporous materials (KINPOR) ( BOF project: DEF/09/ERC/403 )		
<b>Price-class</b>	58 €/nodeday (+ 0% VAT)		
<b>Pre-billed</b>	0€		
<b>Billing</b>	<b>2810.80</b> €(Expected 4725x0.58=2740.50€)		
<b>WBS-element</b>	<b>Door Wim</b>		
<b>Start date</b>	03/07/2014		
<b>End date</b>	31/12/2014 (163 days)		
<b>Node-days</b>			
<b>requested</b>	4725		
<b>granted</b>	4725		
<b>used</b>	4846.2 (+121.2) (100% used)		
<b>#Jobs</b>	1152		

## 2. General Project Information of the Application

Metal-Organic Frameworks (MOFs) are a new and important class of porous materials with a wide range of possible industrial applications. Due to their large pore volume, they present materials with enormous “surfacearea to volume” ratio, making them of great interest for catalysis, gasstorage, and also sensing applications. In case of the latter type of applications, the sensing aspect often results in a modification of the electronic and/or magnetic structure of the host material. In this project, we will investigate the stability of different magnetic onfigurations of MIL-47/53 type MOFs, to assess the viability of these frameworks as magnetic sensors.

The main focus will go the MIL-47/53 type MOFs with experimentally known magnetic transition(s). Although, such transitions are known, no ab-initio quantum mechanical studies of these aspects have yet been performed for the MOFs studied in this project. Because the MOFs of interest are also part of the class breathing MOFs, the relation between the magnetic configuration (more specifically the intra-and inter-chain coupling terms) and the large-pore/narrow-pore geometry are of interest (application as pressure sensor). By investigating the variation of the magnetic stability as function of the metal-centre in the MOF (e.g. Sc-Ti-V-Cr) it becomes possible to predict/propose suitable metal centres for specific sensing applications.

### 3. Resources Used per User

User	Id	#jobs	Node days	% node days	Cost €(excl. VAT)
Danny	40201	209	2400.2	49.53	1392.12
Michael	40479	943	2446.0	50.47	1418.67
<b>Total</b>		<b>1152</b>	<b>4846.2</b>		<b>2810.79</b>

### 4. Resources per Project/Paper

#### 4.1. Projects by Danny

##### 4.1.1. Accurate MOF Calculations with VASP

<b>Publication</b>	Paper on accurate calculations of MOFs An Ghysels, Danny E. P. Vanpoucke, Kurt Lejaeghere, and Veronique Van Speybroeck		
<b>Status Publication</b>	<b>Draft</b>		
<b># jobs</b>	111		
<b># node-days</b>	1051.83	<b>Cost(excl. VAT)</b>	610.06
<b>Description</b>			
<ul style="list-style-type: none"> <li>• Calculation of barrier-profile</li> <li>• Optimizations for Phonon-based structure optimization</li> <li>• Investigation of hexagonal (monoclinic) and orthogonal (orthorhombic) MIL-47(V) structures</li> </ul>			

##### 4.1.2. The Electronic and Magnetic Structure of Breathing Metal-Organic Frameworks

<b># jobs</b>	86		
<b># node-days</b>	1317.071	<b>Cost(excl. VAT)</b>	763.90
<b>Description</b>			
Preliminary structure optimizations for different spin-configurations MIL-53(V), MIL-53(Al), narrow and large pore			

##### 4.1.3. HI-charges on Biomolecules

<b>Publication</b>	“On the convergence of atomic charges with the size of the enzymatic environment” Danny E.P. Vanpoucke, Julianna Oláh, Frank De Proft, Veronique Van Speybroeck, Goedele Roos <i>Journal of Chemical Information and Modeling.</i>		
<b>Status Publication</b>	<b>Accepted (Jan 2015)</b>		
<b># jobs</b>	10		
<b># node-days</b>	12.025	<b>Cost(excl. VAT)</b>	6.97
<b>Description</b>			
Additional calculations requested by one of the referees, to investigate the DOS of the structures.			

#### 4.1.4. Functionalized Linkers on UiO-66

<b>Publication</b>	Engineering intrinsic light adsorption properties of UiO-66 frameworks Kevin Hendrickx, Danny Vanpoucke, Karen Hemelsoet,...		
<b>Status Publication</b>	<b>Draft</b>		
<b># jobs</b>	2		
<b># node-days</b>	2.55	<b>Cost(excl. VAT)</b>	1.48
<b>Description</b>			
First periodic calculations on UiO-66 with functionalized linkers for Kevin. Structure optimizations, intended to provide starting structures to calculate band-structures and electronic DOS.			

#### 4.2. Projects by Michael

##### 4.2.1. Validity of stoichiometry rules and HSAB theory on NC surfaces

<b>Publication</b>	Paper on stoichiometry (HSAB as separate paper later on) M. Sluydts, K. De Nolf, Z. Hens, V. Van Speybroeck and S. Cottenier		
<b>Status Publication</b>	<b>Planning</b>		
<b># jobs</b>	490		
<b># node-days</b>	1946.7	<b>Cost(excl. VAT)</b>	1129.08
<b>Description</b>			
<ul style="list-style-type: none"> <li>• Ligand adsorption on InP in VASP (1496.6)</li> <li>• Ligand adsorption on ZnSe in VASP (391.7)</li> <li>• Misc: hardness calculations in Gaussian, VASP compilation tests, ... (56.3)</li> </ul>			

##### 4.2.2. Surface deformation of CIS surfaces

<b>Publication</b>	Further research required		
<b>Status Publication</b>	<b>TBD</b>		
<b># jobs</b>	69		
<b># node-days</b>	294.4	<b>Cost(excl. VAT)</b>	170.75
<b>Description</b>			
Surface calibration + NEB TS search in VASP.			

##### 4.2.3. High-throughput screening of point defect properties in Si and Ge

<b>Publication</b>	High-throughput screening of point defect properties in Si and Ge: database and applications		
<b>Status Publication</b>	<b>Submitted</b>		
<b># jobs</b>	61		
<b># node-days</b>	204.9	<b>Cost(excl. VAT)</b>	118.84
<b>Description</b>			
Screening of experimental positions for small defects.			