

Electronic supplementary information (ESI) for manuscript:  
*Phys. Chem. Chem. Phys.*, DOI: 10.1039/c1cp23434j

## H<sub>2</sub> storage in isostructural UiO-67 and UiO-66 MOFs<sup>†</sup>

Sachin Chavan,<sup>1</sup> Jenny G. Vitillo,<sup>1</sup> Diego Gianolio,<sup>1</sup> Olena Zavorotynska,<sup>1</sup>  
Bartolomeo Civalleri,<sup>1</sup> Søren Jakobsen,<sup>2</sup> Merete H. Nilsen,<sup>2</sup> Loredana Valenzano,<sup>3</sup>  
Carlo Lamberti,<sup>1\*</sup> Karl Petter Lillerud,<sup>2</sup> Silvia Bordiga<sup>1</sup>

<sup>1</sup> Department of Inorganic, Physical and Material Chemistry, NIS Centre of Excellence, and INSTM reference center, University of Turin, Via P. Giuria 7, I-10125 Torino, Italy

<sup>2</sup> inGAP centre of Research-based Innovation, Department of Chemistry, University of Oslo, Sem Saerlandsvei 26, N-0315 Oslo, Norway

<sup>3</sup> Department of Physics, Michigan Technological University, 1400 Townsend Dr, Houghton, MI 49931-1295, USA

---

<sup>†</sup> This work is dedicated to Cesare Pisani, suddenly disappeared few weeks ago, taken by his passion on our Alps. He has been a guide for us in science and life. We will never forget him.

\* Corresponding authors: C. Lamberti Tel: +39011-6707841 Fax: +39011-6707855; E-mail: carlo.lamberti@unito.it

## Adopted Zirconium Basis-Set.

### Zr\_all\_electron\_dovesi\_unpub

```
40 8
0 0 9 2. 1.
    3450660.8    0.000034
    467601.94    0.000322
    92314.514    0.0021
    21992.52     0.0112
    6082.9917    0.0475
    1915.2715    0.157
    676.43927    0.3524
    263.00267    0.4238
    106.89395    0.1593
0 1 7 8. 1.
    7730.9357    -0.000356    0.000918
    1743.6542    -0.00657     0.00895
    515.55964    -0.0586     0.0557
    176.18824    -0.1469     0.219
    67.946738    0.2212     0.4536
    29.173149    0.6893     0.397
    13.001228    0.2629     0.1064
0 1 6 8. 1.
    177.67018    0.00399    -0.0124
    59.986876    -0.0365    -0.0757
    24.185965    -0.3385    0.0838
    9.9783433    0.1865     0.9961
    4.3099261    0.9971     1.2441
    1.7492066    0.2468     0.308
0 1 3 8. 1.
    3.8653       -1.595     -0.1149
    1.739        -0.364     0.514
    0.7875       4.9455     1.3848
0 3 6 10. 1.
    297.855      0.00597
    87.4716      0.0474
    31.5134      0.1925
    12.3703      0.4114
    4.9738       0.4381
    1.957        0.1588
0 1 1 2. 1.
    0.33848 1.0 1.0
0 3 2 2. 1.
    2.6978 0.08308
    0.9959 0.34899
0 3 1 0. 1.
    0.413544 1.0
```