Abstract Submitted
for the MAR16 Meeting of
The American Physical Society

## Understanding and controlling the water stability of MOF-74[1]

SEBASTIAN ZULUAGA, Wake Forest University , ERIKA FUENTES, KUI TAN, University of Texas at Dallas, FENG XU, JING LI, Rutgers University, YVES CHABAL, University of Texas at Dallas, TIMO THONHAUSER, Wake Forest University — Metal organic framework (MOF) materials in general, and MOF-74 in particular, have promising properties for many technologically important processes. However, their instability under humid conditions severely restricts their practical use. In this work, we show that this instability and the accompanying reduction of the $CO_2$ uptake capacity of MOF-74 under humid conditions originate in the dissociation of water molecules at the metal centers. In turn, the reduction in the $CO_2$ uptake capacity occurs as the metal centers are occupied by the remaining OH groups after the water molecules dissociate. It follows that the reduction in $CO_2$ uptake depends on the catalytic activity of MOF-74 towards the water dissociation reaction $H_2O \rightarrow OH+H$. On the other hand, we show that—while the water molecules themselves do only have a negligible effect on the crystal structure of MOF-74—the OH and H products of the dissociation reaction can significantly weaken the MOF framework and lead to the observed crystal structure breakdown. With this knowledge, we can now propose a way to suppress this particular reaction and therefore control the stability of the system under humid conditions.

[1] This work was supported in full by DOE Grant No. DE-FG02-08ER46491

Sebastian Zuluaga
Wake Forest University

Date submitted: 13 Oct 2015

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