Abstract Submitted
for the MAR09 Meeting of
The American Physical Society

Smart nanoporous preconcentrator of explosives based on MOF5[1]
KHORGOLKHUU ODBADRAKH[2], JAMES LEWIS, WVU — We present investigations of interactions of explosive molecules RDX and TATP with metal organic framework MOF-5, using DFTY based ab-initio simulation method FIREBALL. Energetics studies in bulk shows that only one of the binding sites of RDX in MOF-5 suggested by quantum chemistry calculations confirm. The absorption site is on a linker of the framework through 2-(OH) bond. However, surface interactions are stronger, with significantly higher binding barriers. We confirmed two adsorption sites on the surface: one with the linker and the other on a connector of the framework through 3-(OH) bonds. The stronger interactions on the surface suggest importance of size, and surfaces of MOF nanoparticles in precontentrating the explosive molecules in the framework. Ab-initio Molecular Dynamics simulations show that the absorption of the RDX in MOF-5 is highly sensitive to temperatures, suggesting high diffusion rates for the explosive molecules at room temperature.

[1]NSF EXP-LA
[2]corresponding author

Khorgolkhuu Odbadrakh
WVU

Date submitted: 21 Nov 2008 Electronic form version 1.4