

## Materials Science and Technology Division

### "Ab-initio studies of interactions of High Explosive Molecules with Metal Organic Frameworks"

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HTML/4515, Room 265

#### **Abstract:**

In this work, we report our investigations on physisorptions of high explosive (HE) molecules 1,3,5-trinitro-s-triazine, or cyclotrimethylene trinitramine (RDX) and triacetone triperoxide (TATP) by an isorecticular metal-organic frameworks (IRMOF IRMOF-1 and 8. IRMOFs are predicted to act as preconcentrators for explosive molecules or other adsorbates due to their high porosity and selectivity through changeable organic linkers. We choose IRMOF-1 as a benchmark test case for further investigations of IRMOF-HE interactions, and IRMOF-8 as simple variation from the IRMOF-1. We use the density-functional theory based code to estimate physisorption energies for the RDX molecules both interior and on surfaces of IRMOF-1 cages. The code uses atomic orbitals to express electronic wave functions with finite cut-off lengths. We use the Becke form of the exchange interactions with a Lee-Yang-Parr correlation interactions for all of the calculations presented here. Forces for each atom are determined using a variation of the Hellmann-Feynman Theorem.

Our calculations show that the RDX molecules interact more strongly with the exterior IRMOF-1 surface than the interior, suggesting an important role of steric hindrance inside periodic IRMOF-1 cages. For IRMOF-8, RDX yields several physisorption type binding configurations, while TATP remains more inert to interactions at zero temperature. We extended our investigations to molecular dynamics simulations at room temperature to see if any trapping configurations of HE molecules result from the configurations at zero temperature.

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