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Interaction of RDX Explosive Molecules with Metal-Organic[1] KHORGOLKHUU ODBADRAKH[2], JAMES LEWIS, West Virginia University — We have studied interactions of cyclotrimethylene trinitramine (RDX), a highly energetic explosive's molecule, with metal-organic framework of composition Zn_4O (1,4-benzenedicarboxylate)$_3$ (MOF-5), within *ab initio* density functional theory method. The structures were optimized with the Fireball atomic orbital basis sets to a good agreement with experimental values. Optimal surface geometries have been obtained for MOF-5-RDX system and first principles estimates of the binding energies, charge transfer, and activation barriers are given.

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