

Abstract Submitted
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Adsorption of TNT, DNAN, NTO, FOX7 and NQ onto Cellulose, Chitin and Cellulose Triacetate. Insights from Density Functional Theory Calculations GUIDO TODDE, SANJIV JHA, GOPINATH SUBRAMANIAN, Univ of Southern Mississippi, MANOJ SHUKLA, Engineer Research and Development Center, Vicksburg, MS 39180, USA — Insensitive munitions (IM) like DNAN (2,4-dinitroanisole), NTO (3-nitro-1,2,4-triazol-5-one), NQ (nitroguanidine) and FOX7 (1,1-diamino-2,2-dinitroethene) reduce the risk of accidental explosions due to shock and high temperature exposure. These compounds are used as replacement for TNT (2,4,6-trinitromethylbenzene) and RDX (1,3,5-hexahydro-1,3,5-trinitro-1,3,5-triazine). Unfortunately they are more soluble than TNT or RDX, hence they can easily spread in the environment and get dissolved by precipitation. Due to the abundance of cellulosic biomass in the environment it is important to investigate the adsorption of these new contaminants onto cellulose and cellulose derivative surfaces. Using Density Functional Theory methods we have studied the adsorption of TNT, DNAN, NTO, NQ and FOX7 onto cellulose I α and I β , chitin and cellulose triacetate. The solvent effect on the adsorption was also investigated. Our results show how all contaminants are adsorbed onto chitin and cellulose I α . FOX7 is very weakly absorbed onto cellulose I β which is mainly found in wood and ramie fibers.

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