Molecular modeling and simulation of explosive nanocontainer

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Molecular modeling of explosive nanocontainer was studied using various simulation methods, e.g. Grand Canonical Monte Carlo (GCMC), classical and Reactive Molecular Dynamics (MD), and Density Functional Theory (DFT). Encapsulation of energetic material, i.e. Nitromethane (NM) in this study, inside carbon based nanocontainer was used for this study. Each of simulation method was employed to take into account the interpretation of controlled model systems; the amount of loading materials (GCMC), capping method of CNT and modeling (classical MD), energy release (DFT), and burst of nanocontainer (Reactive MD). From (5, 5) to (20, 20) arm chair carbon nanotube was used in GCMC study, and (20, 20) arm chair CNT was selected since it can load proper amount of NM. In classical MD, it shows that 209 NMs can be encapsulated inside the capped 6.6nm length of (20, 20) CNT. Finally, explosion dynamics and mechanism inside CNT, which has never been reported, were confirmed using reactive MD.