

## Investigation of core/shell nanoparticles properties by classical molecular dynamic study

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The synthesis of hexolite by Spray Flash Evaporation recently led to the formation of new core/shell highly energetical nanoparticles [1]. The detonation of such compounds produce very small nanodiamonds of high interest for electronics and biomedical applications. It was revealed that such production is influenced by the core/shell ratio, their size and interfaces features (significant at nanometric level). To manage these factors, the determination of the core/shell thermophysical properties and the underlying mechanisms leading to their formation is crucial.

Due to the thermal instability of hexolite core/shell structures, experimental characterization of these systems is challenging therefore a theoretical investigation appeared as a relevant approach to elucidate the properties of these heterogeneous materials under ambient and extreme conditions. This task is undertaken by molecular dynamic simulation, performed using the STAMP code developed at CEA/DAM [2].

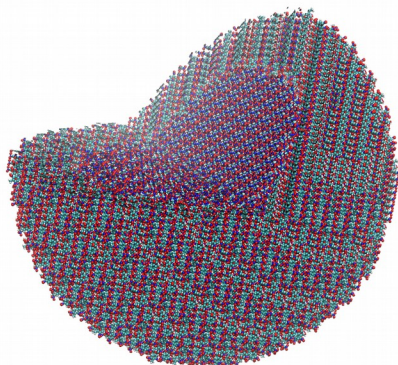
In this work, the development of force fields suitable to describe the core/shell nanoparticles is presented. The validation of the retained potentials is conducted by comparing the structural and thermodynamic properties of the two core shell components, RDX and TNT to the available literature data [3,4]. In a second hand, the study of hexolite component interfaces is conducted to evaluate the influence of the specific spherical geometries against planar ones. Finally, the thermophysical properties for the whole core/shell system are provided.

[1] T. Deckert-Gaudig et al., ChemPhysChem, 18, 175-178 (2017)

[2] N. Pineau et al., STAMP (Simulation Temporelle Atomique-Moléculaire Massivement Parallélisée), Copyright (C) CEA/DAM/DIF 2000-2020.

[3] Choi CS and Prince E, Acta Crystallogr., Sect B 28(9), 2857-2862 (1972)

[4] Vrcelj RM et al., Crys. Growth Des., 3(6), 1027-1032 (2003)



**Figure 1** : Typical modelling of core/shell structures (core RDX, shell : TNT).