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研究论文

TATB基PBX结合能和力学性能的理论研究

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摘要 以SCF-MO-AM1方法和MM-COMPASS力场, 对TATB (1,3,5-三氨基-2,4,6-三硝基苯)与系列高聚物组成的PBX(高聚物粘结炸药)尺寸匹配原子簇, 分别进行全优化几何构型计算, 发现两种方法求得的结合能存在良好的线性关系. 对TATB (3×3×4)超晶胞及其与系列氟聚物组成的双组分PBX, 实施COMPASS力场下的分子动力学(MD)周期性模拟计算, 首次求得其弹性系数、模量和泊松比, 发现添加少量高聚物即能有效改善炸药的力学性能.

关键词 1,3,5-三氨基-2,4,6-三硝基苯(TATB) 高聚物粘结炸药(PBX) 结合能 力学性能 分子动力学

分类号

Theoretical Study on Binding Energies and Mechanical Properties of TATB-based PBX

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Abstract The SCF-MO-AM1 method and MM-COMPASS force field have been applied to the calculation on TATB (1,3,5-triamino-2,4,6-trinitrobenzene) and a series of PBX (Polymer Bonded Explosive). A great deal of parameters of structures and properties including binding energies of PBX were obtained using full geometry optimization on the basis of atomic cluster matching size model. It is found that there is good linear relation between binding energies calculated by AM1 and MM methods. Atomistic molecular dynamics (MD) has been used to simulate mechanical properties of TATB and a series of PBX. Elastic coefficients and effective isotropic elastic constants, such as tensile module, bulk module, shear module, and Poisson's ratio were determined at room temperature and pressure. The results indicate that elastic properties of TATB can be greatly improved by adding a little amount of polymer.

Key words TATB (1 3 5-triamino-2 4 6-trinitrobenzene) polymer bonded explosive (PBX) binding energy mechanical property molecular dynamics (MD)

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