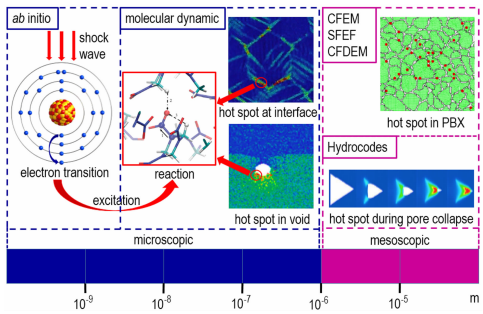
On the Energy & Safety Contradiction of Energetic Materials and the Strategy for Developing Low-sensitive High-energetic Materials

Energy and safety are two most important properties of energetic materials (EMs), but people generally believe that an essential contradiction inevitably exists between them, namely the contradiction between energy and safety (E& S contradiction): the higher the energy, the worse the safety. This article combines some counter examples to discuss the contradiction.

ZHANG Chao-yang

Chinese Journal of Energetic Materials,2018,26(1): 2−10

Lssue of 'Hot-Spot' in Energetic Materials: Recent Progresses of Modeling and Calculations

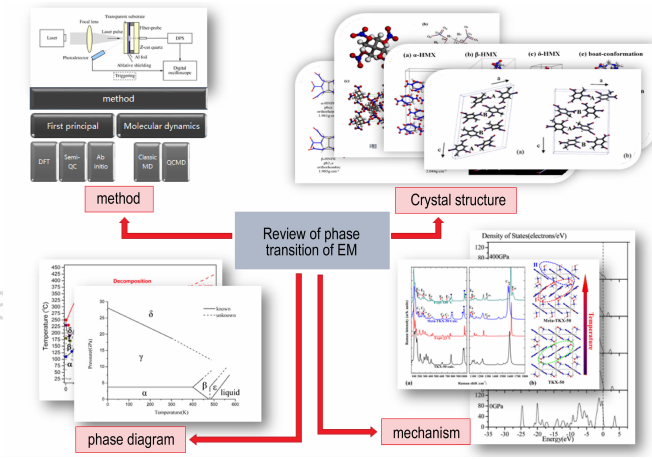


The recent progresses of hot-spot theories in microscopic scale and mesoscopic scale respectively are reviewed.

ZHONG Kai, LIU Jian, WANG Lin-yuan, ZHANG Chao-yang

Chinese Journal of Energetic Materials,2018,26(1): 11−20

Review on the Phase Transition of Energetic Materials

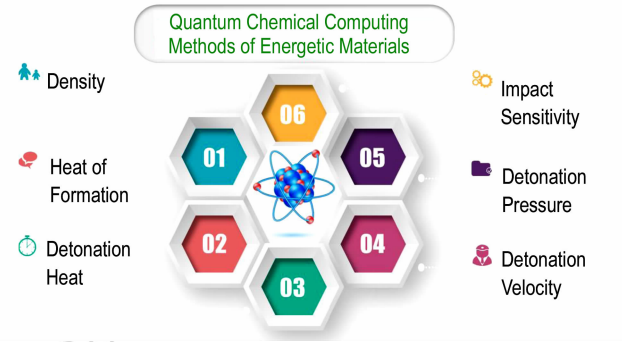


The related research methods that usually used to study the phase transition of energetic materials were reviewed.The commonly used experimental techniques of thermal analysis, ultrahigh pressure and shock loading, as well as many first-principle method and molecular dynamics theoretical simulation research methods with their application scope were introduced. The phase transition characteristics and corresponding phase distributions of some materials under static and shock loading conditions were summarized. The phase transition mechanism revealed by high-precision theoretical simulation investigation of some popular energetic materials was reviewed.

XU Wei-sen, YUAN Jiao-nan, ZHANG Xiu-qing, HU Yan-fei, TIAN Xin, REN Hai-chao, JI Guang-fu, ZHAO Feng

Chinese Journal of Energetic Materials,2018,26(1): 21−33

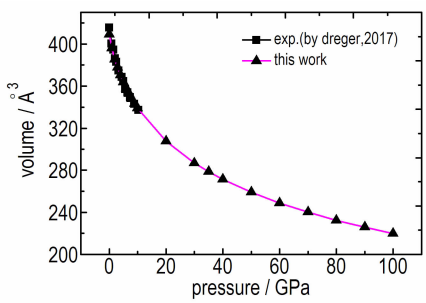
Overview on the Quantum Chemical Methods for Energetic Materials



The basic theory of quantum chemistry was summarized and the calculation methods of key parameters of energetic materials were discussed in detail. The characteristics and applicable scope of these methods were compared. In addition, the application of CHEETA, EXPLO5 and other computing software in the field of energetic materials were briefly introduced. Finally, 20 kinds of new high nitrogen molecules were designed and their physicochemical properties and energetic parameters were estimated by using above-mentioned quantum chemistry methods.

HE Piao, YANG Jun-qing, LI Tong, ZHANG Jian-guo
Chinese Journal of Energetic Materials,2018,26(1): 34-45

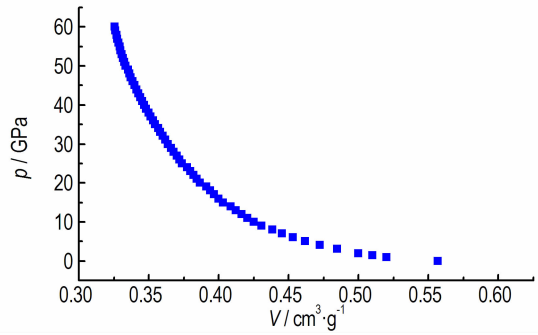
Structural, Mechanical and Electronic Properties of Dihydroxylammonium 5, 5′-Bistetrazole-1, 1′-diolate (TKX-50) under High Pressures: A First-principles Study



The structure, mechanical properties, intermolecular interactions and electronic properties of dihydroxylammonium 5,5′-Bistetrazole-1,1′-diolate(TKX-50) under high pressure are thoroughly studied based on the accurate prediction of pressure-volume relationship.

ZONG He-hou, ZHANG Wei-bin, LI Hua-rong, ZHANG Lei
Chinese Journal of Energetic Materials,2018,26(1): 46-52

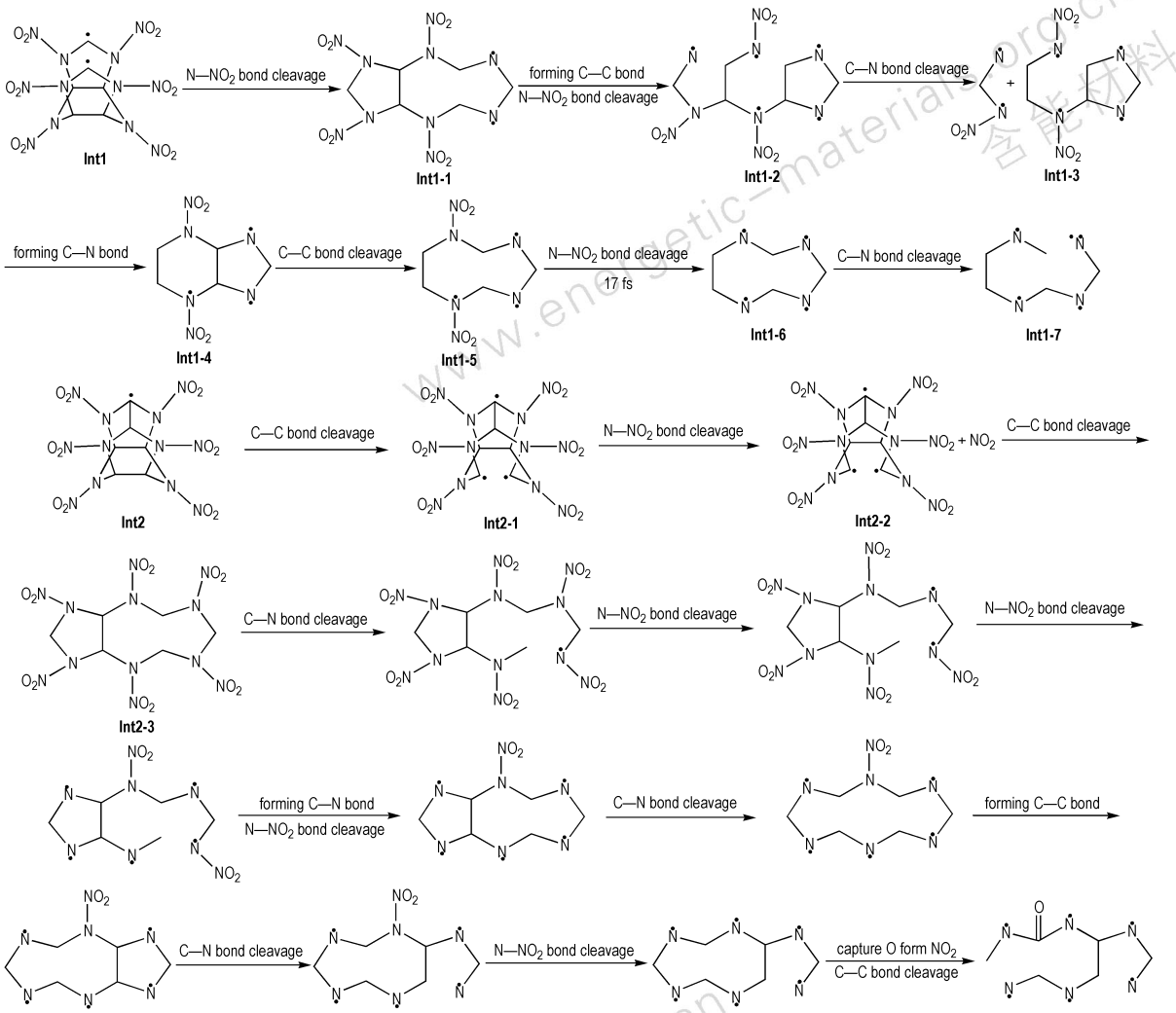
Isentropic Compression Loading Locus of α-RDX Based on Its Self-consistent Force Field



Based on the self-consistent force field-phonon (SCFF-phonon) approach with the anharmonic effect, the isentropic compression loading locus for α-RDX was obtained, covering a full pressure range (i.e., ambient to the high pressures at von Neumann spike) to which the explosive are suffered from.

SONG Hua-jie, LI Hua, ZHANG Ping, YANG Yan-qiang, HUANG Feng-lei
Chinese Journal of Energetic Materials,2018,26(1): 53-58

Ab Initio Molecular Dynamics Studies on the Decomposition Mechanisms of CL-20 Crystal under Extreme Conditions

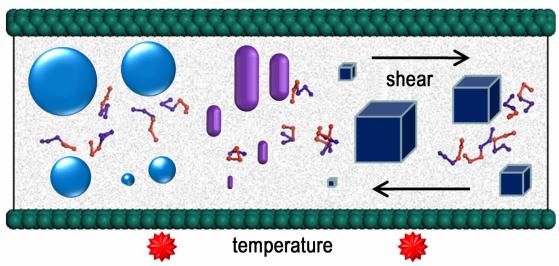


XIANG Dong, WU Qiong, ZHU Wei-hua

***Chinese Journal of Energetic Materials*,2018,26(1): 59-65**

The whole decomposition process of CL-20 during the NVT simulation were analyzed.

DPD Simulations on the Effect of Nanoparticle Shapes, Sizes, Contents and Gradations on the Viscosity of Energetic Suspensions

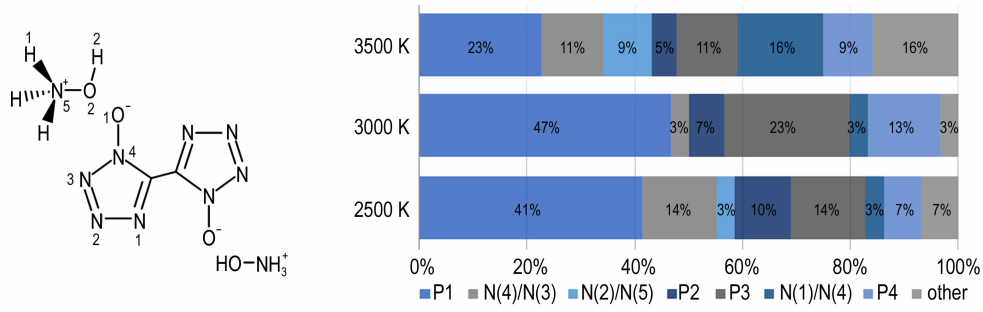


ZHOU Yang, LI Yi-xue, QIAN Wen, HE Bi

***Chinese Journal of Energetic Materials*,2018,26(1): 66-74**

The viscosity of TNT suspensions containing RDX nanoparticles is investigated by the DPD method. Besides the effect rule of nanoparticle on TNT suspensions, a revised Einstein viscosity theory model that can predict the viscosity of the nano-fluid and general fluid is provided.

Molecular Simulation on the Nitrogen Generation in Thermal Decomposition of TKX-50

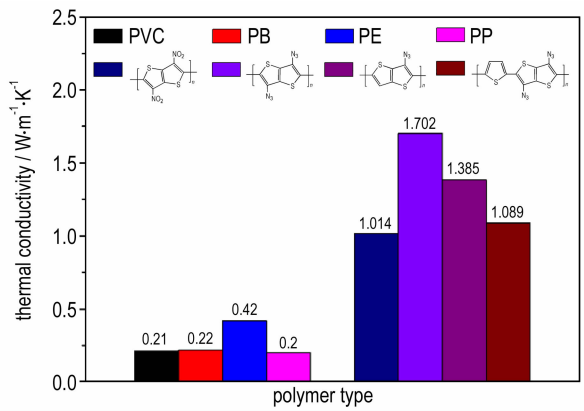


YU Yi, ZHANG Lei, JIANG Sheng-li, WANG Xing, ZHAO Han-yue, CHEN Jun

Chinese Journal of Energetic Materials, 2018, 26(1): 75-79

The decomposition mechanism of TKX-50 was studied using ab initio molecular dynamics simulation.

Prediction on Thermal Conductivity of Energetic Polymers

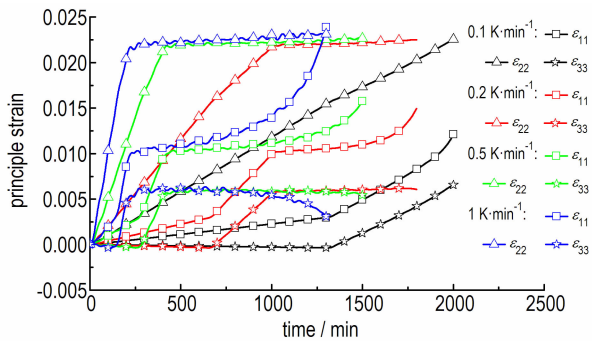


Based on the analyses of the structures, properties, and thermal conduction mechanism of conjugated polymers, several energetic conjugated polymers are designed by introducing energetic group —NO_2, —N_3 and—ONO_2 on the conjugated polymer structures. The thermal conductivities of new designed energetic conjugated polymers are calculated by Askadskii's group contribution method.

GUO Xu-dong, TAN Bi-sheng, HUANG Zhong

Chinese Journal of Energetic Materials, 2018, 26(1): 80-85

Anisotropic Mechanical Response and Phase Transition of Cooked HMX

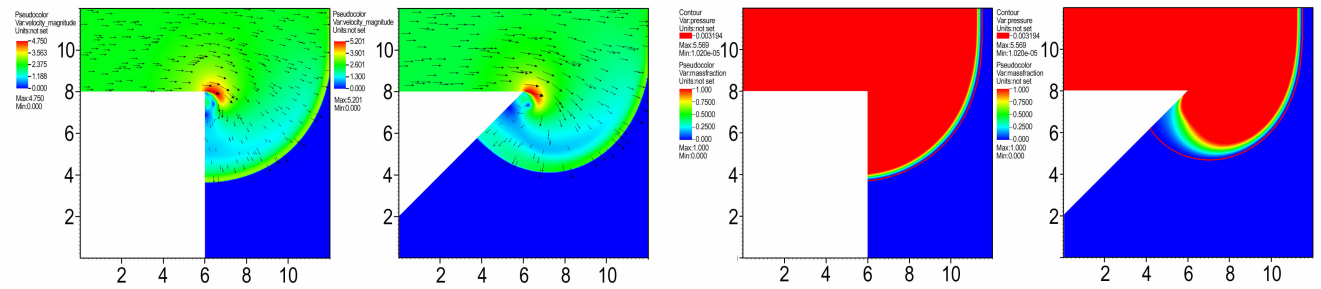


The crystal plasticity constitutive model was developed to investigate the role of $\beta \rightarrow \delta$ phase transformation on the deformation mechanisms of HMX single crystal. Simulated phase transition evolutions of HMX under different heating rates were investigated using finite element software ABAQUS.

HU Wei-jia, WU Yan-qing, HUANG Feng-lei

Chinese Journal of Energetic Materials, 2018, 26(1): 86-93

Numerical Simulations of the Corner Detonation of Condensed Phase Explosives

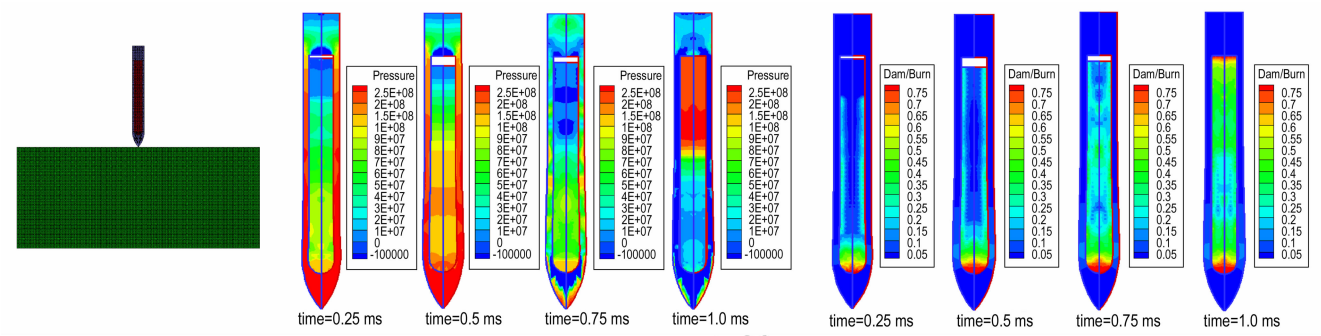


The hybrid detonation formulation of three-dimensional condensed phase explosives is presented based on the multiphase compressible fluid equation and the reaction rate equation. The iteration method of thermodynamic equilibrium for the multiphase detonation mixed reaction zone is built and an efficient detonation parallel software is developed. The feasibility of the physical model, the numerical method and the program module are verified by comparative experiments.

WANG Xing, JIANG Sheng-li, ZHAO Han-yue, YU Yi, ZHANG Lei, CHEN Jun

Chinese Journal of Energetic Materials, **2018**, **26**(**1**): **94-100**

Numerical Simulation on the Dynamic Damage of PBX Charges Filled in Projectiles During Penetrating Thin Concrete Targets



Three kinds of damage forms, void collapse damage, explosive crystal fragmentation and adhesive debonding damage were introduced to viscoelastic constitutive model to explore the mechanical response and damage distribution of casting PBX charge in the penetration process of projectile. The mechanical response of low strain rate to middle and high strain rate of casting PBX at different temperatures was fitted, and the mechanical damage response of explosive in penetrating concrete target of projectile with charge was simulated by the dynamic finite element software.

ZHANG Xin-yu, WU Yan-qing, HANG Feng-lei

Chinese Journal of Energetic Materials, **2018**, **26**(**1**): **101-108**