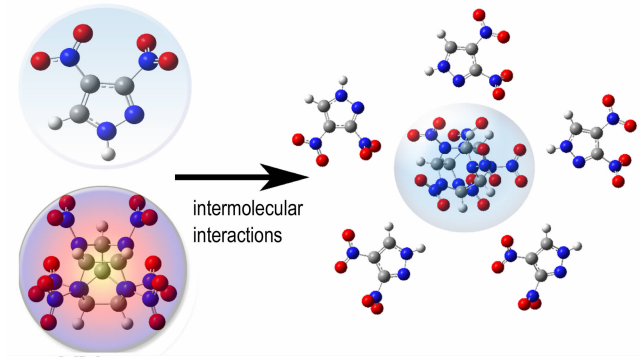
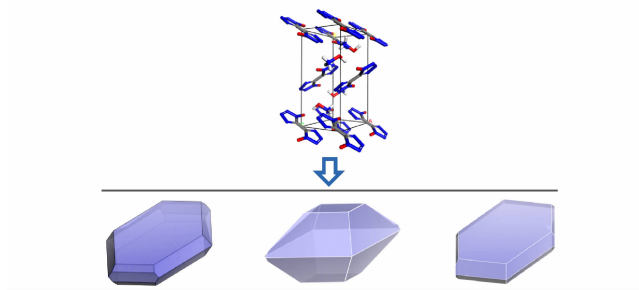
**Theoretical Investigation on the Intermolecular Interactions of 3,4-Dinitropyrazole/Hexaazaisowurtzitane**




ZHU Shuang-fei, ZHANG Shu-hai, GOU Rui-jun, HAN Gang
*Chinese Journal of Energetic Materials*,2018,26(3): 201-209

To explore the changes of CL-20 sensitivity and provide helpful insights on the preparation of DNP/CL-20 mixture explosives, DNP/CL-20 complex was investigated by quantum chemistry methods.

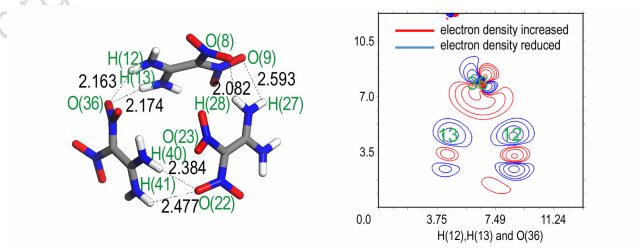
**Crystal Morphology Prediction of Dihydroxylammonium 5,5′-Bistetrazole-1,1′-diolate Under Different Growth Conditions**



LIU Ying-zhe, BI Fu-qiang, LAI Wei-peng, YU Tao, MA Yi-ding, GE Zhong-xue
*Chinese Journal of Energetic Materials*,2018,26(3): 210-217

The growth morphologies of dihydroxylammonium 5,5′-bistetrazole-1,1′-diolate crystal under different conditions, i.e. vacuum, solvent, and additive, were predicted with the aid of attachment model, which is in reasonable agreement with the experiments.

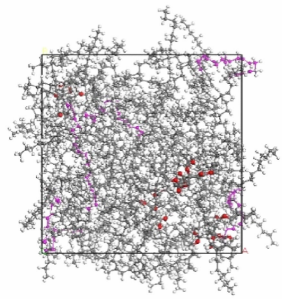
**Quantum Chemical Study on Effects of Intermolecular Interactions in FOX-7 Clusters on the Dissociation of FOX-7**




LI Xiao-dong, XU Zhe, YAN Xiang, LIU Lei, WANG Heng, WANG Jing-yu
*Chinese Journal of Energetic Materials*,2018,26(3): 218-222

The research of FOX-7 clusters by using dispersion corrected density functional theory was performed to simulate the existing state of FOX-7 molecule in crystal structure. Electron density difference at binding sites in FOX-7 clusters was plotted. The intermolecular interaction of condensed phase FOX-7 and its effects on the decomposition mechanism of FOX-7 were also described.

**Molecular Dynamics Simulation on Compatibility of SBS Toughened Paraffin Wax/Plasticizer Blends**

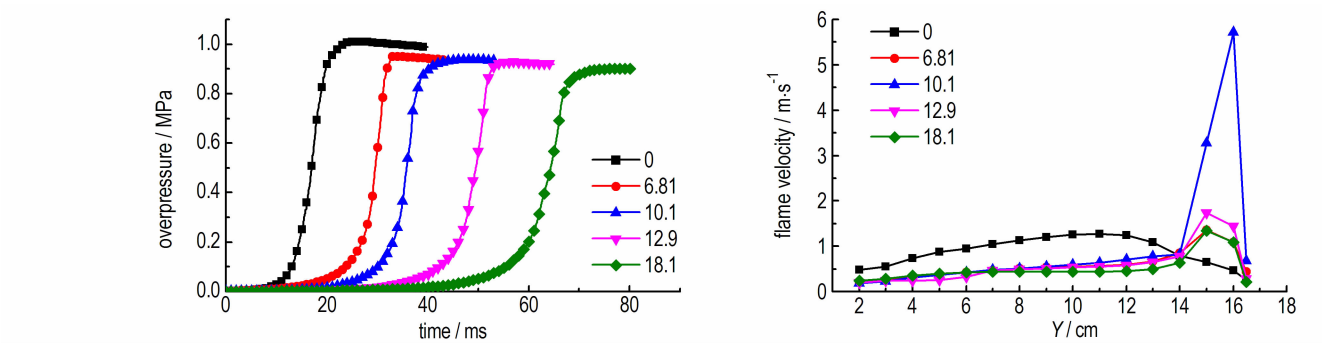


LI Deng-hui, LI Li-jie, LAN Guan-chao, CHEN Yu, JIN Shao-hua, CHEN Shu-sen

***Chinese Journal of Energetic Materials*,2018,26(3): 223-229**

The compatibility of styrene-butadiene-styrene block copolymer(SBS) toughened paraffin Wax with dibutyl phthalate(DBP), dioctyl sebacate(DOS), nitroglycerin(NG) and acetyl tribuyl citrate(ATBC) was studied by molecular dynamics method, and the intermolecular interactions between them were discussed.

**Numerical Simulation of the Influence of Partical Size on Explosion Parameters of *n*-Heptane/Air Mixtures**

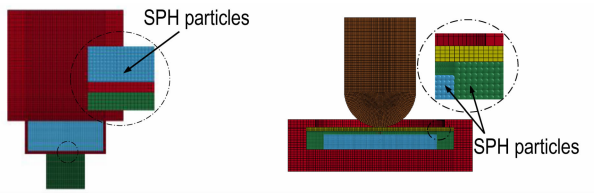



WANG Jing-xin, ZHANG Qi, CHEN Teng-fei

***Chinese Journal of Energetic Materials*,2018,26(3): 230-236**

The effect of the droplets size of *n*-heptane ($C_7H_{16}$) on the explosion parameters was numerically simulated with the vapor-liquid concentration of 80 g·m$^{-3}$.

**Comparative Analysis of Two Algorithms for Simulating the Impact Response Characteristics of Explosives**

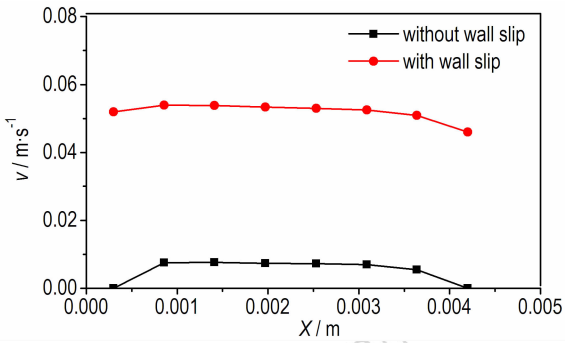


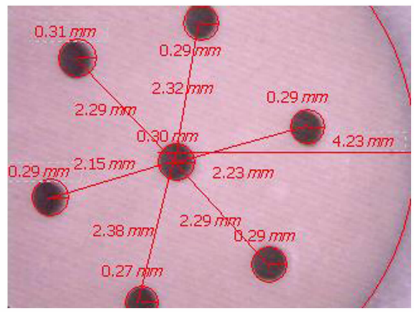

ZHANG Meng-hua, RUAN Wen-jun, YU Yong-gang

***Chinese Journal of Energetic Materials*,2018,26(3): 237-242**

The FEM-SPH coupling algorithm was used to complete the numerical simulation of the drop test and the Steven test. Results were compared with FEM to indicate the advantages of the FEM-SPH coupling algorithm.

## Numerical Simulation of Nitroguanidine Gun Propellant in Channel Considering Wall Slip Correction



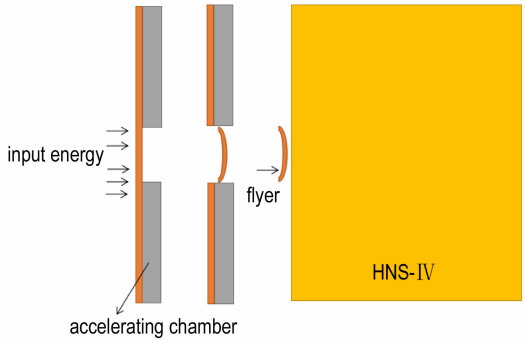




ZHU Chun-jiu, NAN Feng-qiang, HE Wei-dong, SHEN Wan-wu

*Chinese Journal of Energetic Materials*, 2018, 26(3): 243-247

The mechanism of the wall slip of nitroguanidine propellant dough was studied. The pressure field and velocity vector field of nitroguanidine gun propellant in different extrusion process are analyzed by the FEM method. Compared with experiment sizes, the errors of simulation sizes are small.

## Numerical Simulation of the Factors Affecting the Ignition Threshold of an Exploding Foil Initiator

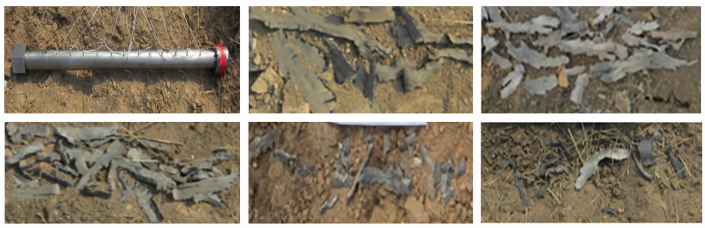


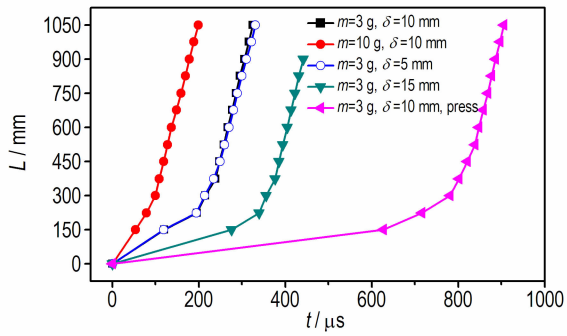

QIAN Shi-chuan, GAN Qiang, REN Zhi-wei, CHENG Nian-shou, FENG Chang-gen

*Chinese Journal of Energetic Materials*, 2018, 26(3): 248-254

The process that bridge foil driven flyer to detonate HNS-Ⅳ was simulated by ANSYS/AUTODYN software. The influence of bridge foil thickness on flyer speed was studied, and the influences of bridge area width, flyer material, flyer thickness and accelerating chamber length on EFI ignition threshold were investigated.

## Experiment Study on the Influence Factors of the Deflagration to Detonation Transition for DNTF-based Explosives



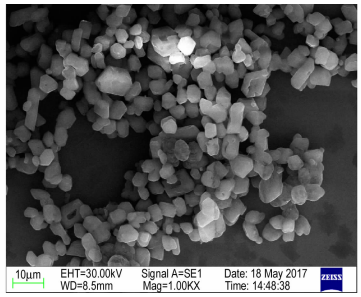


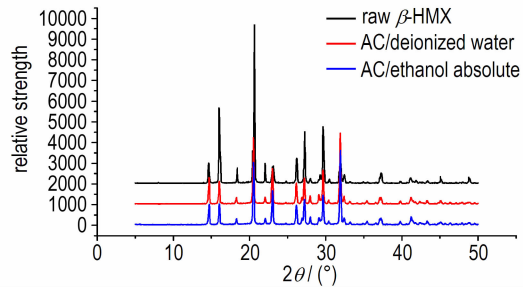

FENG Xiao-jun, TIAN Xuan, ZHAO Juan, FENG Bo

*Chinese Journal of Energetic Materials*, 2018, 26(3): 255-259

The effect of ignition charge mass, thickness of DDT tube and molding way on the performance of deflagration to detonation transition (DDT) for DNTF-based composite explosive was investigated by the coaxial ionization probe test technology.

**Ultrafine High Quality HMX Prepared by Ultrasonic Assisted Spray Method and Its Crystal Type Control**

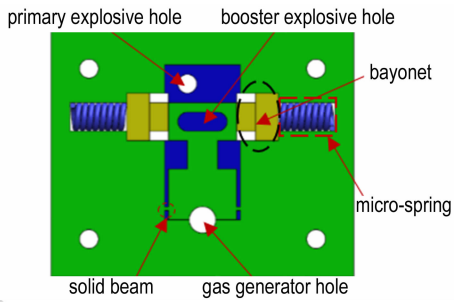


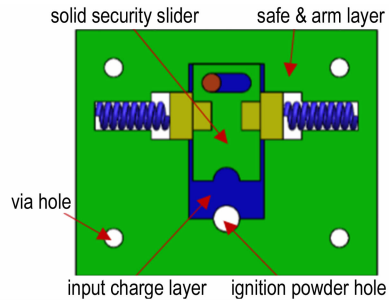




XU Wen-zheng, PANG Zhao-ying, WANG Jing-yu, PING Chao
*Chinese Journal of Energetic Materials*, **2018**, **26**(**3**): **260-266**

The superfine HMX was prepared by an ultrasonic assisted spray recrystallization refining method. The effects of atomization rates, solvent and non-solvent type and temperature etc. on the particle morphology and crystal type of HMX were studied.

**Design, Fabrication and Actuation Performance of PyroMEMS Safe and Arm Device Based on Silicon Double Solid Beams**

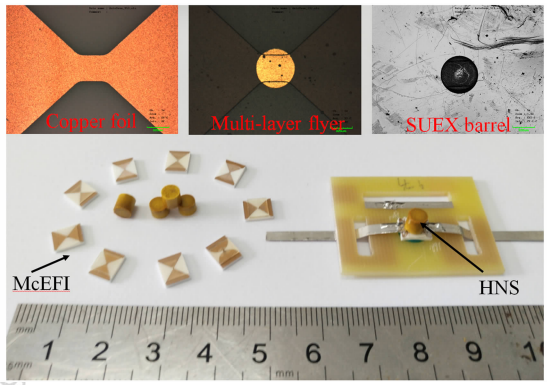



HOU Gang, ZHU Peng, LI Yu, SHEN Rui-qi, YE Ying-hua
*Chinese Journal of Energetic Materials*, **2018**, **26**(**3**): **267-272**

APyroMEMS S & A device based on silicon double solid beams was designed and fabricated. Its main characteristics include that large displacement, integrated batch production, and it does not need to use inertia force to disarm the device. This PyroMEMS S & A device can realize safe and arming functions and can satisfy the miniaturization and high reliability requirements of modern safety system.

**Effect of Barrel and Multilayer Flyer on the Performances of Micro Chip Exploding Foil Initiator**

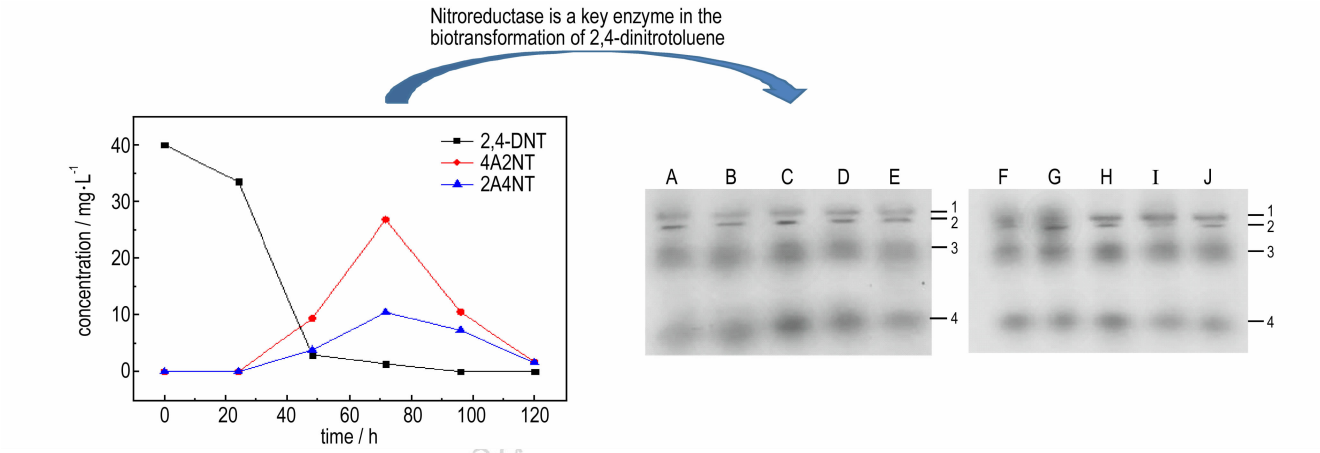



The exploding foil initiator was integrally prepared through MEMS process. Bridge foil of Cu with 0.4 mm×0.4 mm×4.6 μm ($L\times W\times H$) and Parylene C/Cu multilayer flyer were prepared by sputtering and chemical vapor deposition. Three kinds of SUEX epoxy thick film barrels were prepared using ultraviolet lithography technology. The influence of firing voltage and barrel size on the velocity of multilayer flyer was studied by photonic doppler velometer(PDV), and the detonation tests of HNS explosives were carried out.

CHEN Kai, XU Cong, ZHU Peng, FU Shuai, WU Li-zhi, SHEN Rui-qi, YE Ying-hua

***Chinese Journal of Energetic Materials*,2018,26(3): 273-278**

**Biotransformation of 2,4-Dinitrotoluene and Properties of Nitroreductase by *Rhodobacter Sphaeroides***




The important intermedimates, 2-amino-4-nitrotoluene and 4-amino-2-nitrotoluene, produced during the biotransformation of 2,4-dinitrotoluene by *Rhodobacter sphaeroides* were studied. Nitroreductase is a key enzyme in the biotransformation of 2,4-dinitrotoluene. The pattern of isoenzymes of nitroreductase was analyzed using native-PAGE method.

WANG Shou-yan, BAI Hong-juan, ZHAO Ting-ting, KANG Peng-zhou

***Chinese Journal of Energetic Materials*,2018,26(3): 279-284**