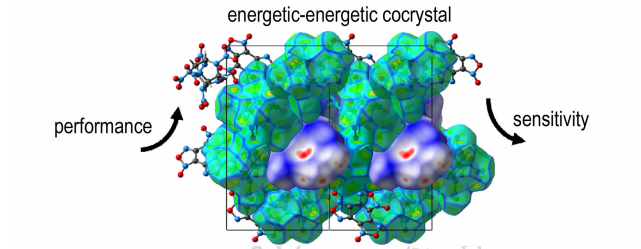
Theoretical Study on Thermodynamic Stability and Detonation Performance of CL-20 and Its Cocrystal

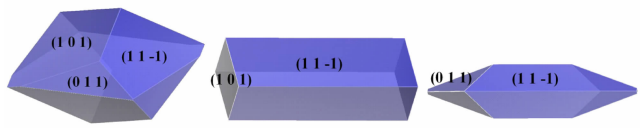


ZHANG Lei, ZHAO Yan-hong, JIANG Sheng-li, YU Yi, WANG Xing, ZHAO Han-yue, LI Chong-yang, CHEN Jun

Chinese Journal of Energetic Materials, 2018, 26(6): 464-470

By performing both first-principles and statistical physical simulations, the effect of intermolecular interaction on the nature of α-, β-, γ-, ζ-, ε- polymorphs of CL-20 crystal, BTF crystal, and CL-20/BTF cocrystal explosives were revealed.

Prediction of Crystal Morphology of FOX-7 in H_2O/DMF Solvents

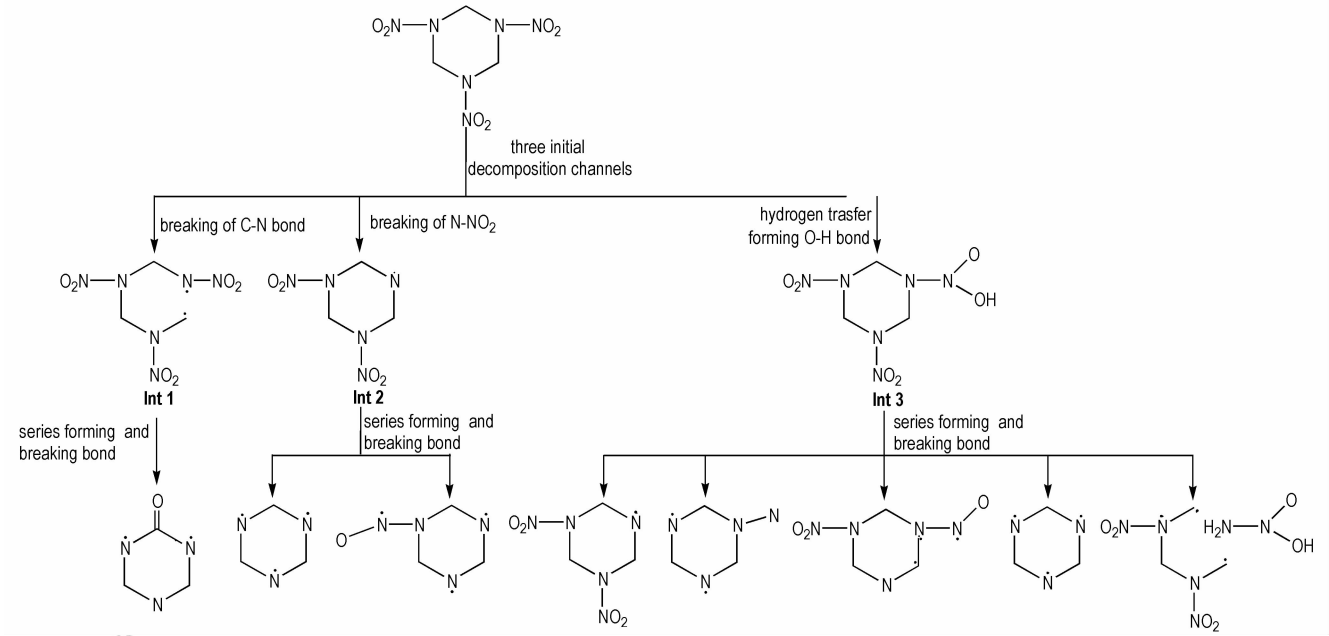


LIU Ning, ZHOU Cheng, WU Zong-kai, SHU Yuan-jie, WANG Bo-zhou, ZHAO Qiang-li, WANG Wen-liang

Chinese Journal of Energetic Materials, 2018, 26(6): 471-476

The crystal morphologies of FOX-7 in H_2O/DMF solvents at different temperatures were predicted by modified attachment energy (MEA) model. The intermolecular interactions of crystal surface and solvent molecules were also studied.

Decomposition Mechanisms of α-RDX Crystal Under High Temperature Coupled with Detonation Pressure by Ab Initio Molecular Dynamics Simulations

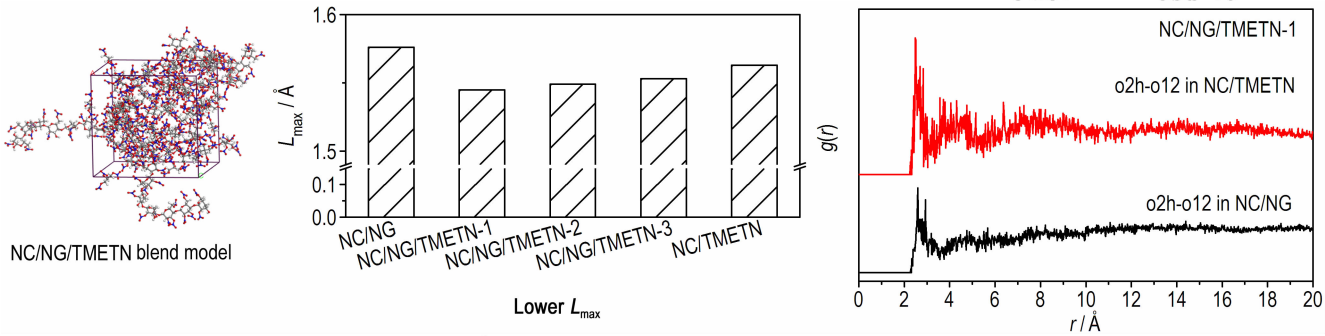


XIANG Dong, WU Qiong, ZHU Wei-hua

Chinese Journal of Energetic Materials, 2018, 26(6): 477-482

The complete decomposition process of α-RDX crystal at 3000 K coupled with 34.5 GPa was studied via. ab initio MD simulation method.

Simulation on the Properties of TMETN/NG Mixed-plasticizers/NC Blends

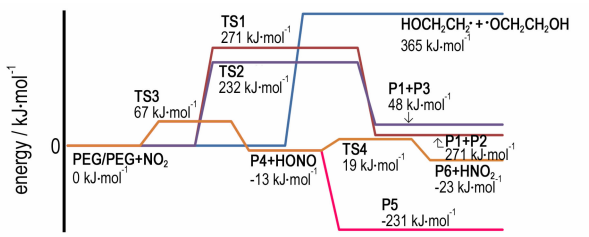


CHEN Jing, LIU Meng, HE Qi-wen, MA Yi-ding, XU Kang-zhen, FAN Xue-zhong

Chinese Journal of Energetic Materials, 2018, 26(6): 483-488

Taking nitrocellulose (NC) as binder, five kinds of blending models which contain 2-methyl-2-[(nitrooxy)methyl]propane-1,3-diyl dinitrate(TMETN), nitroglycerin(NG), and three kinds of TMETN/NG mixed-plasticizers with different mass ratio were constructed. The interactions, mechanical properties, radial distribution functions, and maximum trigger bond (O—NO_2) length (L_{max}) etc. parameters for each blending system were simulated by molecular dynamics method using materials studio software.

Molecular Simulation Study on the Aging Mechanism of Polyethylene Glycol

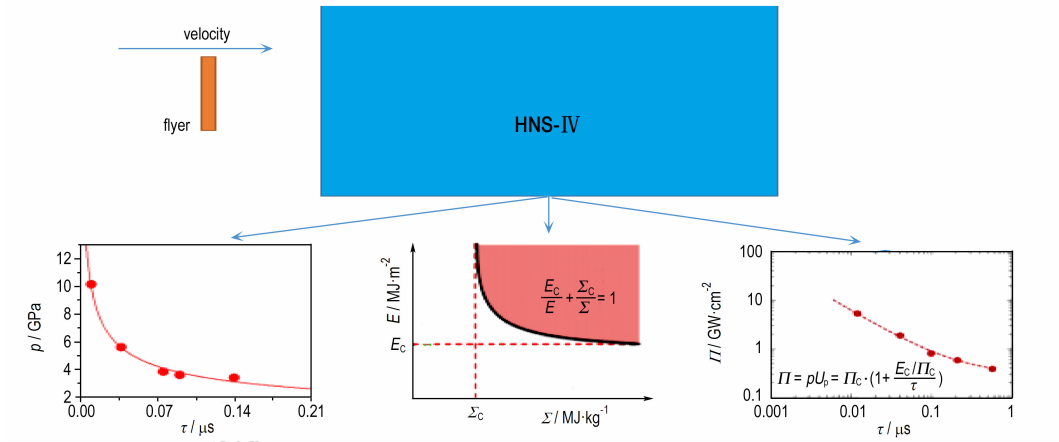


PEI Li-guan, DONG Ke-hai, LI Wen-zuo, CHENG Jian-bo, TANG Yan-hui, ZHAO Peng

Chinese Journal of Energetic Materials, 2018, 26(6): 489-494

Based on the B3LYP method of density functional theory (DFT) and canonical variational transition state theory combined with a small-curvature tunneling correction (CVT/SCT), the molecular simulation and calculation for the aging reaction type of PEG molecule in the presencee of PEG unimolecule and NO_2 molecule were carried out.

Study on One-dimensional Shock Initiation Criterion of HNS-Ⅳ Explosive

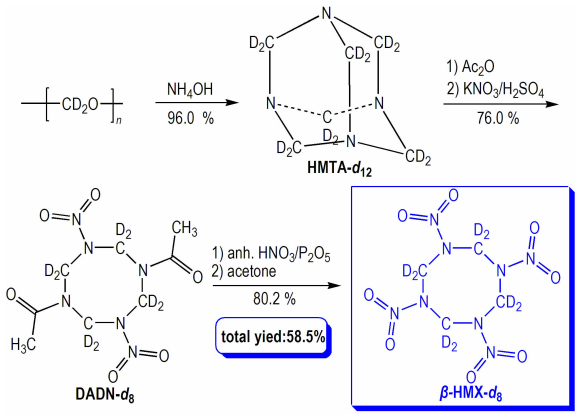


QIAN Shi-chuan, GAN Qiang, REN Zhi-wei, CHENG Nian-shou, FENG Chang-gen

Chinese Journal of Energetic Materials, 2018, 26(6): 495-501

The initiation of HNS-Ⅳ explosive is achieved by giving the flyer velocity. In this way, different initiation criteria such as p-τ criterion, James criterion and Π-τ criterion are studied.

Synthesis of β-Phase Deuterated Octogen (β-HMX-d_8)

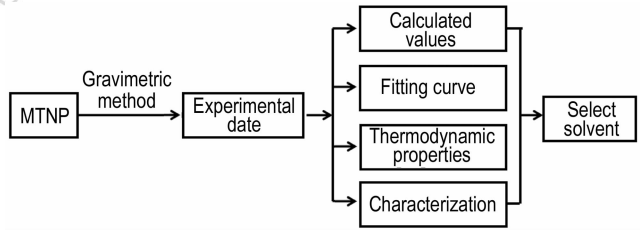


HU Gang, LEI Jian-lei, NING Hong-li, LI Hao, SUN Guang-ai, GONG Jian, BAI Liang-fei, YANG Hai-jun

Chinese Journal of Energetic Materials, 2018, 26(6): 502-510

Based on the synthesis technology of non-deuterated HMX using paraformaldehyde as raw material, β-deuterated octagon (β-HMX-d_8) was successfully synthesized.

Crystallization Thermodynamics of 1-Methyl-3, 4, 5-trinitropyrazole

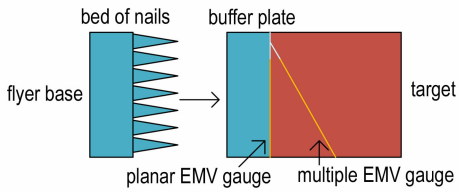


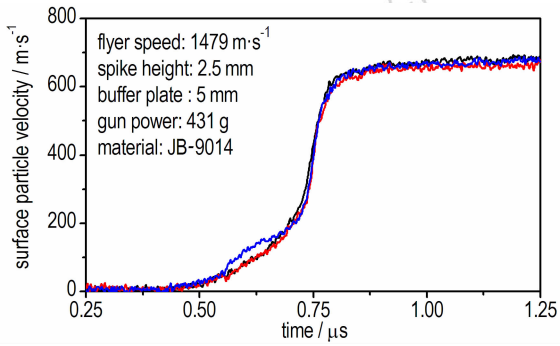
GUO Heng-jie, CAO Duan-lin, DANG Xin, CHAI Xiao-xiao, FAN Li-hong, LI Yong-xiang

Chinese Journal of Energetic Materials, 2018, 26(6): 511-516

The solubility of 1-methyl-3, 4, 5-trinitropyrazole (MTNP) in different solvents was determined by the gravimetric method. The Apelblat equation and vant't Hoff equation were used to correlate the solubility data. The standard enthalpy of dissolution, standard entropy of dissolution, standard Gibbs free energy of dissolution, solid-liquid surface tension and surface entropy factor of MTNP were estimated by the experimental data. The product was characterized. The optimum solvent was selected.

Experimental Technology of Quasi-isentropic Compression Process Generated by a Graded Areal Density Flyer System Under Impact Loading



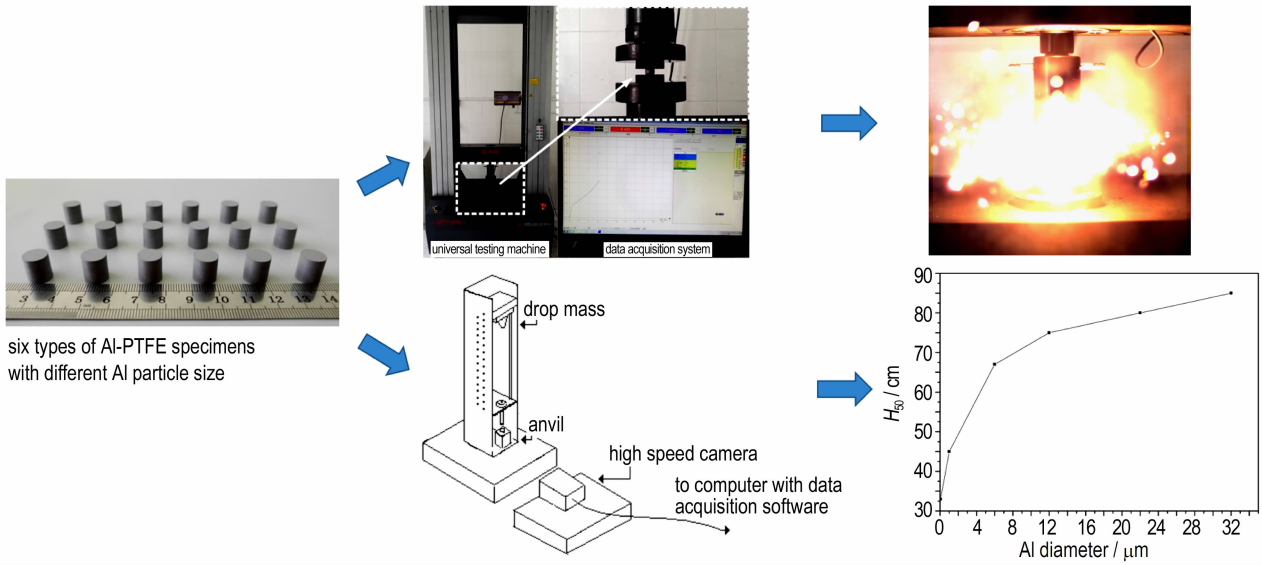


ZHAO Kang, ZHANG Xu, LIU Jun-ming, ZHONG Bin, ZHANG Rong

Chinese Journal of Energetic Materials, 2018, 26(6): 517-523

The JB-9014 explosive target was subjected to quasi-isentropic compression generated by a PTEF flyer which termed 'bed of nails' and the impact loading device. The particle velocity was captured by Al-based multiple electromagnetic particle velocity gauge technique.

Effect of Al Particle Size on the Quasi-static Compression Reaction and Drop Hammer Impact Sensitivity of Al-PTFE

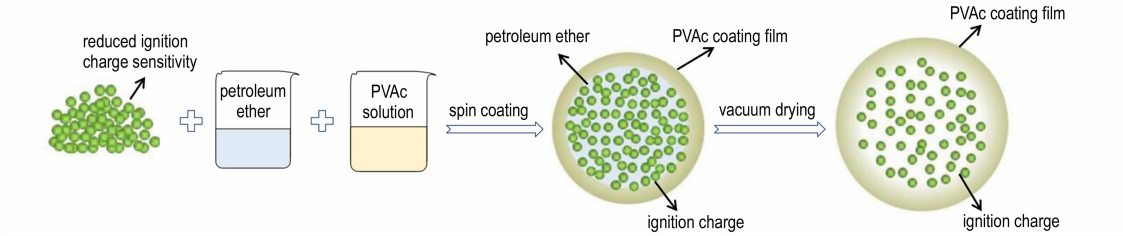


WU Jia-xiang, LI Yu-chun, FANG Xiang, WANG Huai-xi, FENG Bin, WU Shuang-zhang

Chinese Journal of Energetic Materials, 2018, 26(6): 524-529

Six types of Al-PTFE reactive material specimens with different Al particle size were prepared by molding sintering method and were comparatively tested by universal testing machine and drop hammer machine, and observed by high-speed photography instrument. The stress-strain curves and impact sensitivity data of different specimens were obtained, and the effect of Al particle size on the quasi-static compression mechanical properties and impact sensitivity of Al-PTFE was analyzed.

Ignition Performance of the High Energy Chemical Igniter Coated with a PVAc Elastic Microsphere

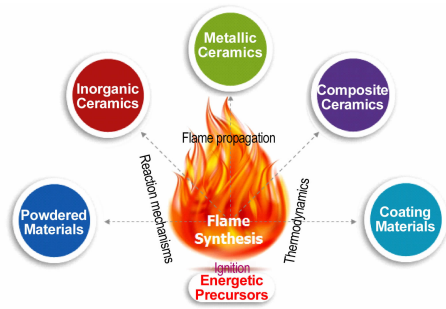


A high energy chemical igniter coated with a PVAc elastic microsphere was developed. In the process of drying, the petroleum ether was volatilized to make the coated film expand and the igniter powder bulk, which improves the specific surface area of igniter. The igniter has a excellent ignition performance and the PVAc elastic microsphere has the advantages of good formability, high toughness and strength. The water proof and oxidation resistance functions of PVAc elastic microsphere also improve the storage stability of the igniter.

LIU Wen-jin, CHENG Yang-fan, LU Song-lai, HAN Ti-fei, WANG Quan, SHEN Zhao-wu

Chinese Journal of Energetic Materials,2018,26(6): 530-536

Recent Progress on the Functional Materials Synthesized by High Temperature Self-Propagating Reactions

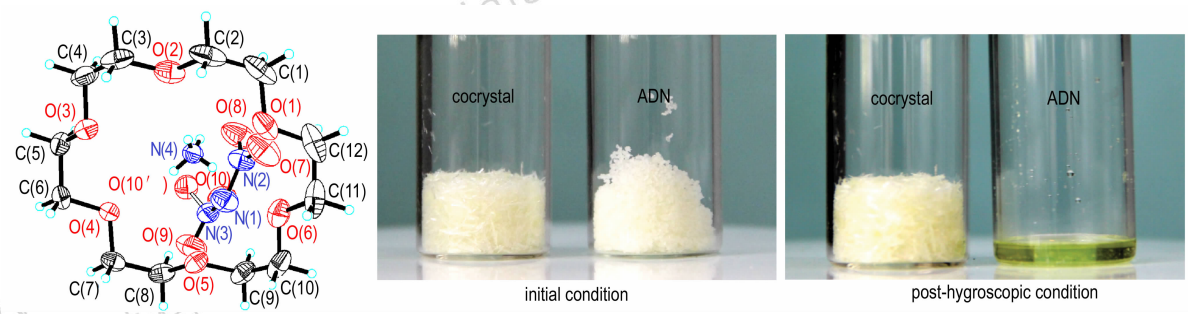


The advances in self-propagating high-temperature synthesis (SHS) technique have been briefly summarized. The components of SHS precursor system and typical SHS products are discussed with more details. The reaction mechanisms, ignition behavior, and thermodynamics are presented as well.

ZUO Bei-lin, LIU Pei-jin, ZHANG Wei-hai, YAN Qi-long

Chinese Journal of Energetic Materials,2018,26(6): 537-544

Preparation and Characterization of ADN/18C6 Cocrystal



The cocrystal of ammonium dinitramide (ADN)/18-crown-6 (18C6) was prepared by solvent evaporation method, and the cocrystal structure was confirmed by SXRD. The hygroscopicity of ADN is dramatically reduced through cocrystallizing with 18C6.

WANG Hao-jing, MA Yuan, LI Hong-zhen, YU Yan-wu, YANG Zong-wei

Chinese Journal of Energetic Materials,2018,26(6): 545-548