EI 收 录 期 刊
中 文 核 心 期 刊
中国科技核心期刊

ISSN 1007—7812
CODEN HUXUFP

火炸药学报

CHINESE JOURNAL OF EXPLOSIVES & PROPELLANTS

(Chin J Explos Propellants)

计算含能材料专刊（Ⅰ）

封面文章：机器学习势在含能材料分子模拟中的研究进展
——常晓雅，文明杰，张迪，王永锦，初庆钊，朱通，陈东平

Vol.46 No.5
2023
中国兵工学会

本刊系《中文核心期刊要目总览》(2020 年版)、国务院《学位与研究生教育重要期刊》、科技部《中国科技论文统计源期刊》(中国科技核心期刊)、中国科学院《中国科学引文数据库》及中国科协《中国学术期刊文摘(英文版)》、美国《化学文摘》(CA)、Scopus 数据库、Ei Compendex 数据库、俄罗斯《文摘杂志》(AJ)、日本 JST China 数据库、美国《乌利希期刊指南(网络版)》(Ulrichsweb)数据库收录源刊。

刊名题写：张爱萍

目　　次

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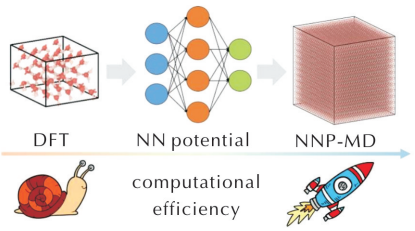
期刊基本参数：CN61-1310/TJ * 1978 * m * A4 * 104 * zh * p * ￥20.00 * 1000 * 11 * 2023-05

Contents

Recent Progress toward Molecular Modeling of Energetic Materials by Using Machine Learning Potential

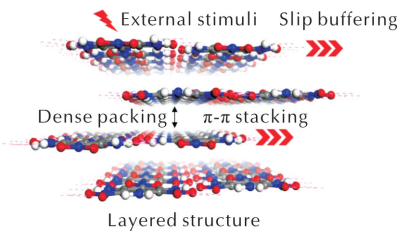


CHANG Xiao-ya, WEN Ming-jie, ZHANG Di, WANG Yong-jin, CHU Qing-zhao, ZHU Tong, CHEN Dong-ping

Chinese Journal of Explosives & Propellants, 2023, 46(5): 361-377.

The data-driven manner embedded in machine learning potential model enables million-atom molecular simulations of energetic materials, maintaining the accuracy of first-principles calculations.

Research Advance on the Design Strategies of Layered Energetic Materials

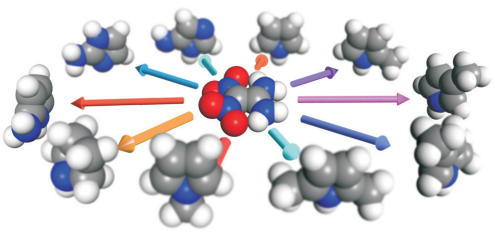


HE Xiao-kai, CAO Yi-lin, LIU Ying-zhe

Chinese Journal of Explosives & Propellants, 2023, 46(5): 378-389.

Layered energetic materials are a class of crystalline energetic materials with layered stacking characteristics formed by planar organic energetic molecules through hydrogen bonds, π-π stacking and other intermolecular interactions. They are potentially low sensitive and high energetic. High stacking coefficient of layered energetic materials helps to increase the crystal density, reduce the free volume, which in turn improve the detonation performance and lower the impact sensitivity. In addition, the interlayer sliding can also act as buffer against the external mechanical stimulation.

Pyrrole and Pyrimidine Derivatives as Possible Electron Donors for Colored Charge-Transfer Complexes with a Weakly Electrophilic Energetic Material, FOX-7: A Theoretical Study



arrows indicate approximate color of the complexes

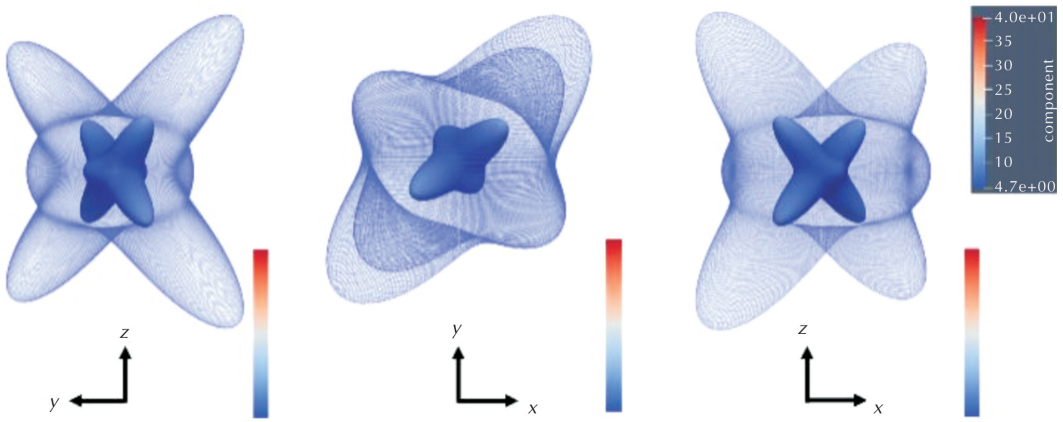
Graphical TOC

Sergey V. Bondarchuk

Chinese Journal of Explosives & Propellants, 2023, 46(5): 390-398.

A number of electron-rich heterocycles are studied as potential reagents for visual colorimetric detection of FOX-7 due to colored charge-transfer complexes formation. The obtained results suggest that pyrrole and pyrimidine derivatives can form such complexes playing the role of electron donors despite a low electrophilicity of FOX-7. Density functional theory calculations, as well as quantum theory of atoms in molecules analysis, suggest stacking binding mode as the most preferable one with the binding energy of about 21—36 kJ/mol.

Effect of London Dispersion Interaction on the Atomic Structure and Elastic Properties of Energetic Molecule Crystals

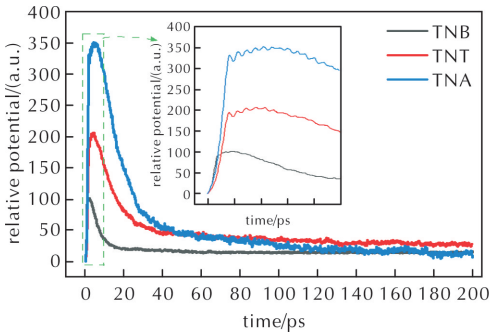


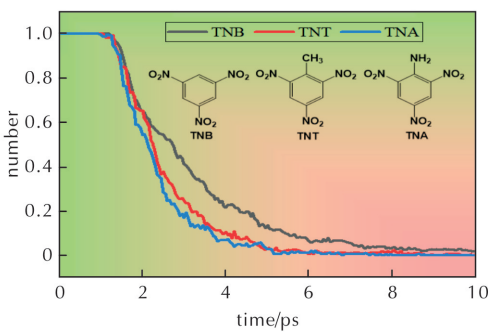
LI Yi-wei, FAN Xiao-jing, WEI Wei, HAN Xu-hui, HE Chun-lin, HU Tao, SHAO Zi-qiang, CHEN Pan

Chinese Journal of Explosives & Propellants,2023,46(5): 399-410.

The non-covalent interactions and elastic tensors of γ-CL-20, TATB and HMX were calculated based on density functional theory (DFT) by adjusting different dispersion correction methods. The effect of dispersion interactions on the elastic tensor of HMX was quantified.

ReaxFF/lg study on the substituent effect upon the thermal decomposition mechanism of nitrobenzene compounds



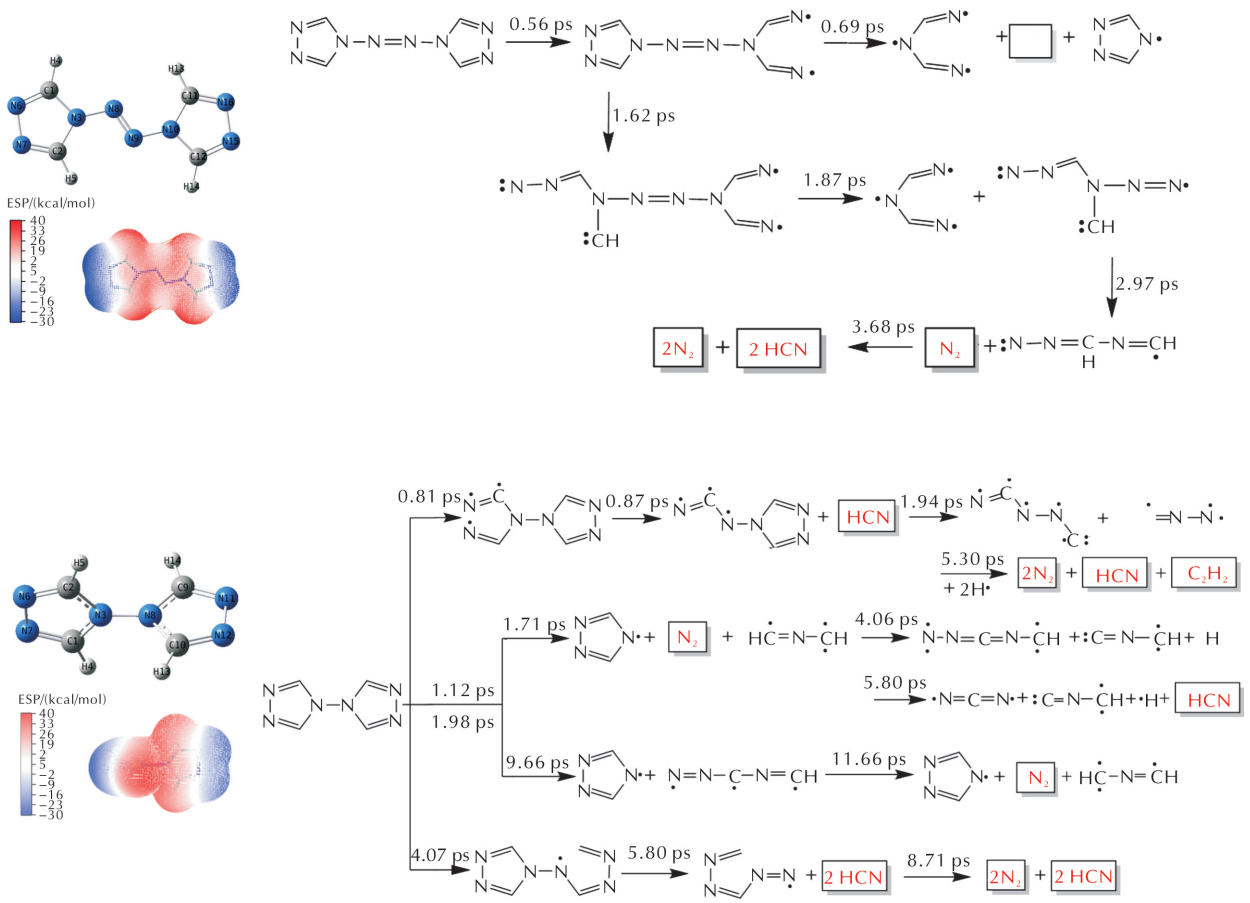


ZHU Shuang-fei, ZHU Rui, ZHANG Shu-hai, LUO Chun-wang, FENG Shang-biao, LIU Guang-rui

Chinese Journal of Explosives & Propellants,2023,46(5): 411-418.

The initial decomposition reaction, product and cluster of the three nitrobenzene compounds were studied by ReaxFF/lg molecular dynamic simulations, and the influence of substituents on the thermal decomposition mechanism of nitrobenzenes was elucidated.

DFT Calculation of Energetic Properties of 4,4′-azo-1,2,4-Triazole (ATRZ) and 4,4′-bi-1,2,4 Triazole (BTRZ)

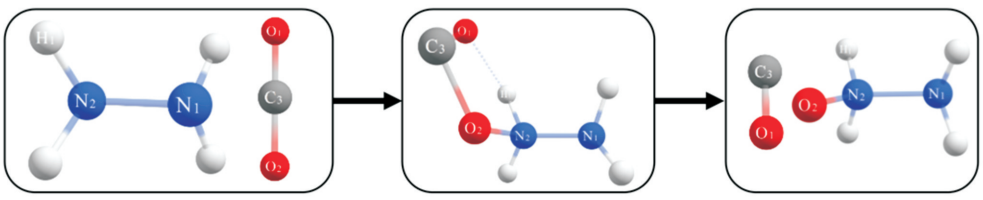


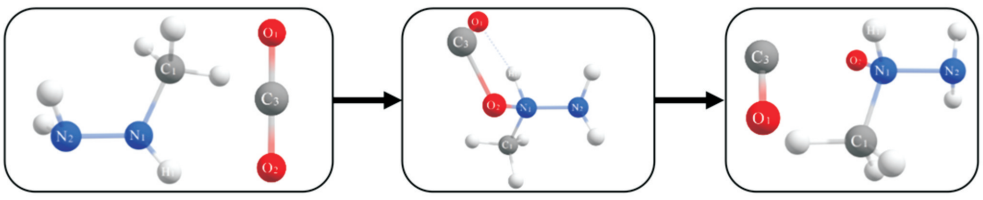
HUANG Xin, ZHANG Pei-pei, BU Shu, HE Xiao-hui, WANG Kun, CHENG Long-jiu

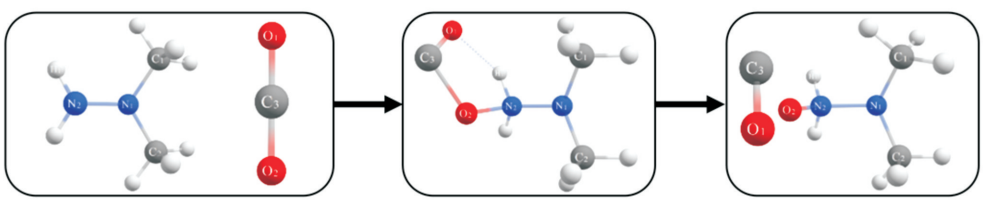
Chinese Journal of Explosives & Propellants, 2023, 46(5): 419-426.

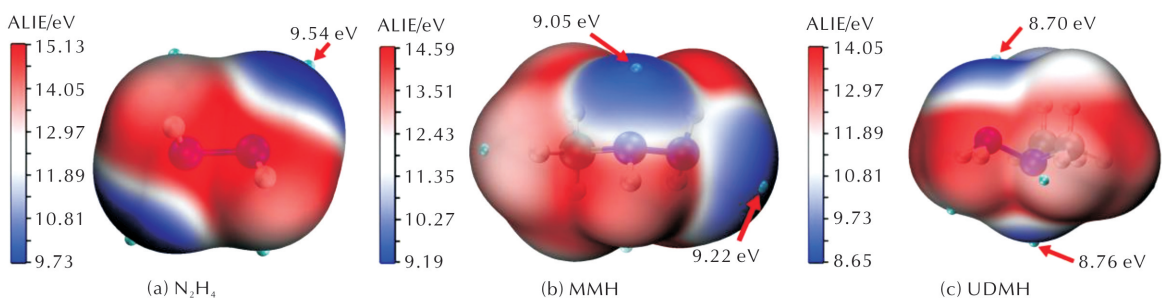
GGA-PBE method with MS-CASTEP was applied to optimize the crystal structures of ATRZ and BTRZ. CPMD method were explored to understand the initial decomposition mechanism of ATRZ and BTRZ at 2000K. Theoretical level of TPSS/6-311++G(3d,2p) was used to calculate the formation enthalpies, explosion pressure and velocity of ATRZ and BTRZ.

Reaction Mechanism Study of Hydrazine Fuels Induced by CO_2 at Low Temperatures





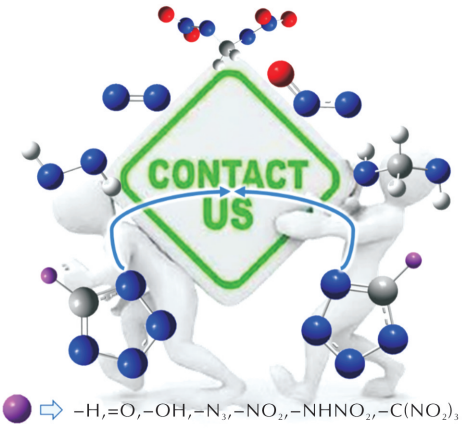




CHEN Rui-zhe, LIU Yong-feng, WANG Long, BI Gui-jun, SONG Jin-ou
Chinese Journal of Explosives & Propellants, 2023, 46(5): 427-435.

Quantum chemical calculations were used to analyze the reaction processes and potential energy surfaces of hydrazine (N_2H_4), methyl hydrazine (MMH) and unsymmetrical dimethyl hydrazine (UDMH) with CO_2 at different temperatures.

Design and Performance Study of Five New Dicyclotetrazole Energetic Compounds

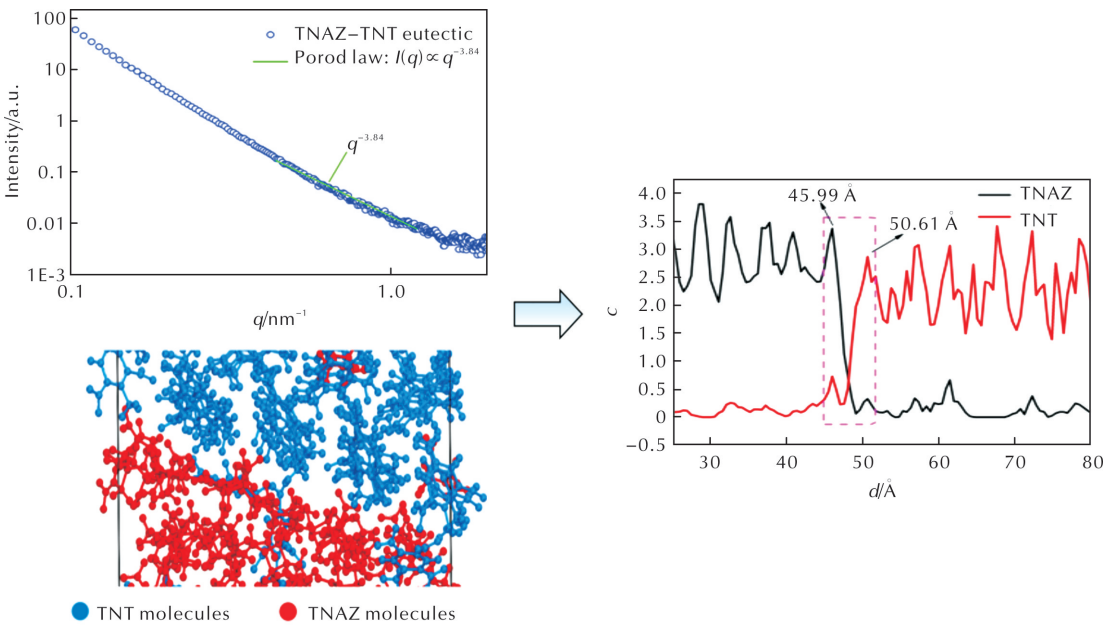


ZHANG Ming-min, JIANG Shuai-jie, ZHANG Li-nan, ZHU Mi-mi, QIN Kai-yi, LIN Qiu-han

Chinese Journal of Explosives & Propellants, 2023, 46(5): 436-440.

By using tetrazole as the parent structural unit, five new groups of bicyclic tetrazolium-containing compounds (A—E) were designed by introducing a variety of high-energy and bridging groups. The electronic properties and detonation performances of the 35 designed compounds were calculated and analyzed using the density functional theory method at B3LYP/6-311G (d, p) level, and their detonation parameters were compared with those of HMX and other explosives.

Microstructure of TNAZ-TNT Eutectic

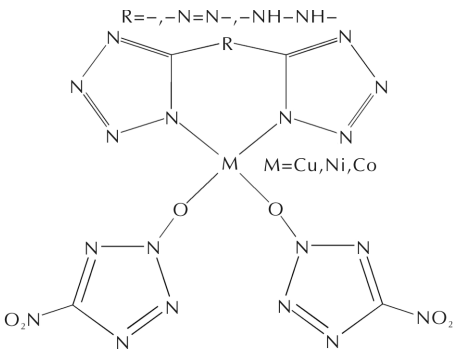


CHEN Ling-yuan, YOU Ting, LIAO Yi-mei, TIAN Qiang, DUAN Xiao-hui

Chinese Journal of Explosives & Propellants, 2023, 46(5): 441-448.

The microstructure of 1, 3, 3-trinitroazetidine (TNAZ)-2, 4, 6-trinitrotoluene (TNT) eutectic was investigated by differential scanning calorimetry (DSC), scanning electron microscope (SEM), X-ray diffraction (XRD), Fourier transform infrared spectrum (FT-IR), small-angle X-ray scattering (SAXS) combined with theoretical simulations.

A New Design Strategy for High-energy Insensitive Metal Complexes: A Combination of All-tetrazole High-nitrogen Ligands, Less Nitro and Oxygen Balance Close to Zero

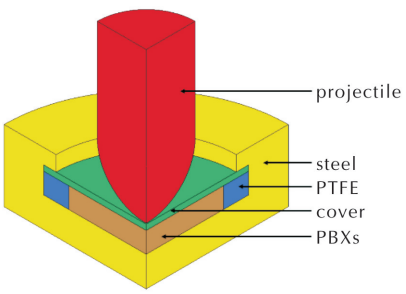


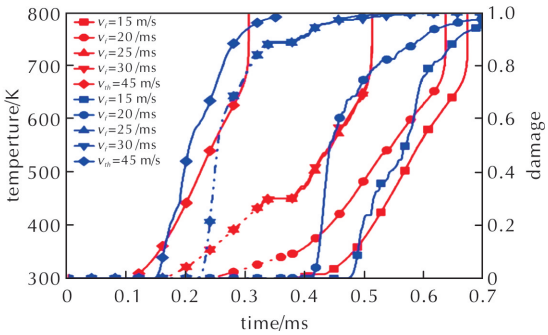
Three series of new energetic metal complexes with higher energy and lower sensitivity than HMX have been designed and predicted by a new strategy: a combination of all-tetrazole high-nitrogen ligands, less nitro and oxygen balance close to zero.

LIU Xuan-xia, CHEN Wei, XU Wei, YAN Gao-jie, WU Qiong, ZHU Wei-hua

Chinese Journal of Explosives & Propellants, 2023, 46(5): 449-455.

Numerical Simulation on Low-velocity Impact Ignition Behavior of PBXs with Damage Accumulation





The mechanical-thermal-chemical coupled model of PBXs considered the asymmetric evolution of microcrack under tension and compression, was used to simulate the ignition behavior of HMX-based PBXs with damage accumulation.

WANG Yi-ming, LIU Rui, CHEN Peng-wan, JIA Lu-chuan, BIAN Yun-long

Chinese Journal of Explosives & Propellants, 2023, 46(5): 456-464.

火炸药学报

公开发行 1978年创刊 月刊
第46卷 第5期(总第231期)

CHINESE JOURNAL OF EXPLOSIVES & PROPELLANTS
(**Monthly, Started in 1978**)
Vol. 46 No. 5 2023 Series No. 231

主管单位:中国科学技术协会
主办单位:中国兵工学会
中国兵器工业第204研究所
编辑出版:《火炸药学报》编辑部
主 编:魏 卫
副 主 编:赵凤起
执行主编:李念念
责任编辑:肖会君
印 刷:西安创维印务有限公司
中国标准连续出版物号:ISSN 1007-7812 CN 61-1310/TJ

Managed by China Association for Science and Technology
Sponsored by China Ordnance Society
The Research Institute No. 204 of the China Ordnance Industry Corporation
Edited by Editorial Board of Journal of Explosives & Propellants
(P. O. Box 18, Xi'an, 710065, China)
Editor-in-Chief: Wei Wei
Deputy Editor-in-Chief: Zhao Feng-qi
Executive Editor-in-Chief: Li Nian-nian

Tel:(029)88291297 E-mail:hzyxb@204s.com http://www.hzyxb.cn 西安市18号信箱(710065) 2023年5月出版 定价:20.00元