Theoretical Study on Molecular Structure and Crystal Band Structure of 4-Amino-1, 2, 4-triazol-5-one

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Abstract: The density-functional theory (DFT) method of the Amsterdam density functional (ADF) was used to calculate the geometry and frequency of 4-amino-1, 2, 4-triazol-5-one (ATO). The calculated results were compared through varying basis sets and relativity effect. The geometry, Mayer bond orders, net charges of atoms, frontier orbital energy and the main atomic orbital percentage were calculated. Results indicate that the basis sets in ADF program have a great influence on the calculation. Results obtained by the basis set of TZP are good conformity with the experimental. The crystal field theory was used to calculate the energy band structure and density of state (DOS) on ATO. The properties of ATO are similar to insulators.

Key words: physical chemistry; density functional theory (DFT); 4-amino-1,2,4-triazol-5-one (ATO); crystal band structure

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Pattern Recognition for Images of Explosion Fireball of **Condensed Explosives Based on Fisher Criterion**

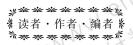
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Abstract: To investigate the feasibility of discriminating explosive type with RGB image of fireball of explosion, the curves of time vs area with intensive light on the images were obtained on the basis of a lot of photographs of explosion of condensed explosive with small dosage (30 g) by the high speed photography, and multi-dimension eigenvector space to describe firelight of explosion of condensed explosives was built by using feature parameters of configurations of curves of area vs time. And finally the linear three-type pattern recognition with optimal eigenvector was made by applying three-type Bayes's decision rule and generalized fisher criterion. The test data of TNT, RDX, HMX were discriminated. Results show that the inaccuracy is 10.07% of pattern recognition built by the training set, while it is 17.48% of pattern recognition with using Jackknifing method in the total sample sets.

Key words: explosion mechanics; light of explosion; Fisher criterion; pattern recognition



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由中国工程物理研究院化工材料研究所、北京理工大学爆炸科学与技术国家重点实验室联合主办,中国工程物理研究 院化工材料研究所承办的 2008 年钝感弹药学术研讨会于 2008 年 3 月 29 日~4 月 1 日在海南省三亚市召开。来自北京理 工大学、南京理工大学、国防科技大学、湖南大学、航天四院、航天六院、二炮军代室、甘肃805厂以及中国工程物理研究院 各研究所的六十余位领导、专家、学者出席了大会,他们就有关钝感弹药技术及研究中产生的新材料、新工艺和新思想进行 了深入的学术交流。此次会议的召开,对推动钝感弹药研究领域的交流与合作,促进钝感弹药的研究发展,将起到积极作用。