

## TATB固体与表面吸附水的相互作用研究

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**摘要** TATB (1, 3, 5-三氨基-2, 4, 6-三硝基苯) 是最著名的耐热钝感炸药; 水在 TATB 表面的吸附作用研究具有理论和实用双重意义。在 B3LYP/6-31G~(\*\*) 水平上, 在对 TATB 晶体 (001) 表面作周期性计算的基础上经基组叠加误差 (BSSE) 校正, 求得 TATB 的表面能为  $-19.90 \text{ kJ}\cdot\text{mol}^{-1}$ , 与实验值良好相符; 首次求得水在 TATB (001) 面的吸附能为  $-10.25 \text{ kJ}\cdot\text{mol}^{-1}$ ; 重点讨论了吸附前后能带和电子结构的变化。

**关键词** [硝基苯](#) [水](#) [吸附](#) [相互作用](#) [电子结构](#)

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## A Study on the Interaction of TATB Solid Surface with Adsorbed Water

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**Abstract** 1,3,5-Triamino-2,4,6-trinitrobenzene (TATB) is the most famous thermo-resistant and insensitive explosive. TATB is always contacted with water in synthesis, uses and storage, especially in making PBX powders. The study of water absorption on TATB surface may have significance both in theory and practice. The periodic calculation of TATB (001) crystal surface was made at DFT-B3LYP/6-31G~(\*\*) level. ON the basis of calibrating of Basis Set Superposition Error (BSSE), the surface energy was given as  $-19.90 \text{ kJ}\cdot\text{mol}^{-1}$ , which is in agreement with the experimental result; the adsorption energy of water on TATB (001) surface ( $-10.25 \text{ kJ}\cdot\text{mol}^{-1}$ ) was presented for the first time. The changes of banding and electronic structure, when water was adsorbed on the (001) surface of TATB crystalline, were discussed.

**Key words** [NITROBENZENE P](#) [WATER](#) [ADSORPTION](#) [INTERACTIONS](#) [ELECTRONIC STRUCTURE](#)

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