Supplementary Information for

Self-assembly of TATB 3D Architectures via Micro-channel Crystallization and formation Mechanism

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Debye-Scherer equation:

To obtain more quantitative information of the prepared TATB nanoparticles, the average particle size can be calculated by inserting the width at half height of the signals into the Debye – Scherrer equation:

$$D_{hkl}=k\lambda/\beta\cos\theta \qquad (1)$$

$$L = 0.89\lambda/(\beta\cos\theta) \qquad (2)$$

where L is the coherence length (nm), β is the full width at half maximum (FWHM) of the peak, λ is the wavelength of the X-ray radiation (1.540598 Å), and θ is the angle of the diffraction peak.

SEM images of TATB prepared by crystallization

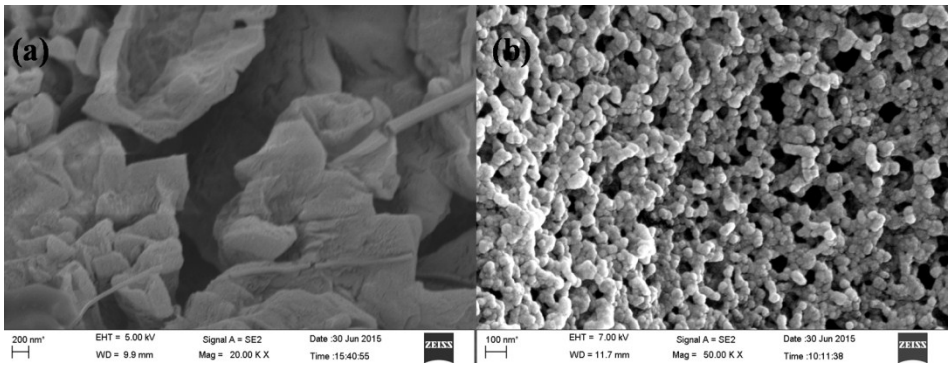

Figure 1S. FESEM images of TATB prepared by solvent and non-solvent crystallization and solvent (a) and solvent and non-solvent crystallization with spray assisted (b).

Until now, few new nanostructure of TATB is reported in literatures. In 2006, we firstly report a novel route to prepared nano-TATB particles with diameter of 60 nm (Propellants, Explosives, Pyrotechnics,2006,5,31). Solvent and non-solvent crystallization is main method to prepare nano-TATB. Figure 1S (a) show morphology of TATB prepared by mixed TATB sulfuric acid with water directly. It displays micro-scale structure. Figure 1S (b) shows morphology of TATB prepared in our previous work.

Nitrogen isotherms

The result shows that chrysanthemum-like TATB 3D architectures have a BET surface area of 20.5 m^2/g, and a pore volume of 0.068 cm^3/g, respectively. Figure 2S (b) indicates a bimodal pore

size distribution, which was calculated from the desorption branch of the isotherm by the BJH method. Small pores for TATB 3D architectures are around 2.3 nm, while the big pores are around 6.4 nm.

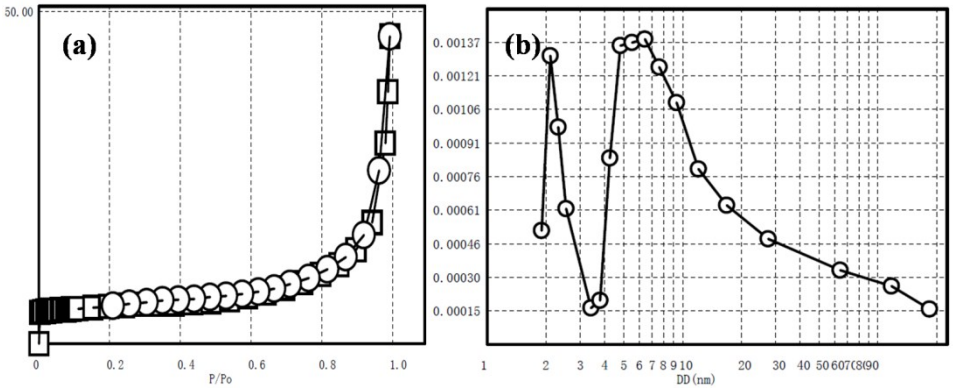

Figure 2S. Nitrogen isotherms and the pore size distribution calculated from desorption branch for chrysanthemum-like TATB 3D architectures.

Hydrogen-bonding of TATB molecular

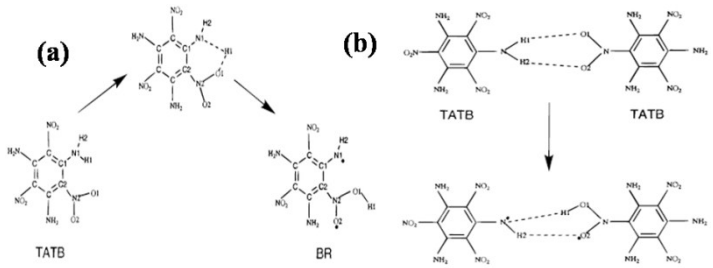

Figure 2S. hydrogen-bonding of TATB molecular (a) intra-molecular hydrogen bond, (b) inter-molecular hydrogen bonds. The lengths of the intra-molecular hydrogen bond range from 1.690 °A to 1.975 A°, while inter-molecular hydrogen bonds are in a range from 1.854 °A to 1.906 A°.