Remarkably Enhanced Photocatalytic Activity in Bi_{1-x}Ba_xFeO₃ Prepared by Sol-Gel Method

<u>Chenlan Zhang</u>¹, Tong Tong¹, Jianguo Chen¹, Dengren Jin¹ and Jinrong Cheng^{1,*} ¹ School of Materials Science and Engineering, Shanghai University NO.99 Shangda Road, Shanghai, China, 200072 *Jinrong Cheng: jrcheng@staff.shu.edu.cn

As a typical multiferroic material, BiFeO₃ (BFO), has exhibited photocatalytic activities under visible light irradiation, thanks to its suitable band gap (2.2–2.8 eV) and good chemical stability. However, the low photocatalytic activity of BFO hinders its commercialization in photocatalytic field for the degradation of organic pollution. Therefore, an important task is to improve the photocatalytic activity of BFO for practical use.

In this paper, a series of nano particles of $Bi_{1-x}Ba_xFeO_3$ (for x = 0,0.01,0.03,0.05,0.10) by Ba^{2+} acceptordoping at A-site were synthesized by a sol–gel method. XRD analysis confirms that Ba ions enter into the lattice, and TEM image shows that Ba^{2+} doping refines the grain whose different size in the range of 30-60 nm. Though testing the photocatalytic degradation of methyl orange (MO), the purpose of our study was to explore the impact of Ba ions on the pure phase BFO, involving the content of Ba ions on the microstructure and surface morphology of the BFO photocatalysts, and the final improvement of their photocatalytic efficiency. We found the optimum concentration of Ba^{2+} doping is x = 0.03. In this condition, $Bi_{1-x}Ba_xFeO_3$ has the highest visible light degradation ratio (81% after 3 hours), which is much higher than that of pure phase BFO (66% after 3 hours).

The smaller particle size which reduces the probability of recombination by reducing the time of charge carriers' migration and the formation of Fe^{4} + or oxygen vacancies should make some influence on enhancement of catalytic efficiency. We also try to make a prediction that Ba2+ serves as an efficient dopant to influence photocatalytic ability through band gap modifications and the change of Fe-O-Fe bond angle by our first-principles calculations.