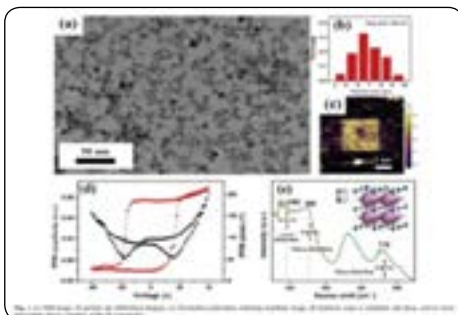


Ferroelectricity in BaTiO₃ nanocrystals: towards future applications

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Ferroelectric materials, which possess a spontaneous and switchable electric polarization below the Curie temperature T_c , are widely used in modern electronics, such as capacitors, nonvolatile memory devices, energy storage applications and nanoelectromechanical systems. As the continuous demand for device miniaturization as well as the rapid development of flexible devices, ferroelectric nanoparticles that served as source materials or fillers to realize energy storage, piezoelectric conversion or memory applications have attracted broad interests in recent years. Ferroelectricity in nanoscale materials is the basis for the design and fabrication of integrated ferroelectric devices. Although a critical ferroelectric size ~ 2.4 nm of BaTiO₃ (BTO) material has been calculated by the first-principles method, no experimental proof of electric polarization has been reported for such small BTO yet. The BTO nanocrystals with particles size from 2.8 nm to 8 nm were prepared by a low-cost, green and scalable sol method. We show that, BTO nanocrystals as small as 2.8 nm are still ferroelectric. Especially, ferroelectric polarization switching image and hysteresis loop show direct evidence for the ferroelectricity of the BTO nanoparticle assembly. With the particle size decreasing from 8.0 to 2.8 nm, the increasing of ferroelectric phases coincides well with the "surface phase" increase from the X-ray photoelectron spectroscopy (XPS) data, showing that surface relaxation is the origin of most non-centrosymmetrical phases in these nanocrystals. Here, we also show high prospect of these soluble ferroelectric nanoparticles in the applications of nanocomposite devices. For instance, as these nanoparticles can achieve a high polarization, we made gradated BTO/PVDF nanocomposite films using the nanocrystal sol (with grain size of 8 nm) and achieved a discharged energy density as high as 19.37 J/cm³.

**Recent Publications:**

1. Hao Y. N., Wang X. H., O'Brien S., Lombardi J., Li L. T. (2016) Flexible BaTiO₃/PVDF gradated multilayer nanocomposite film with enhanced dielectric strength and high energy density. *J. Mater. Chem. C* 3:9740-9747.
2. Hao Y N, Wang X H, Bi K, Zhang J M, Huang Y H, Wu L W, Zhao P Y, Xu K, Lei M, Li L T (2017) Significantly enhanced energy storage performance promoted by ultimate sized ferroelectric BaTiO₃ fillers in nanocomposite films. *Nano Energy* 31: 49-56.
3. Hao YN, Wang XH, Li LT (2014) Highly dispersed SrTiO₃ nanocubes from a rapid sol-precipitation method. *Nanoscale* 6 (14): 7940-7946.
4. Hao YN, Wang XH, Kim JY, Li LT (2014) Rapid Formation of Nanocrystalline BaTiO₃ and Its Highly Stable Sol. *J Am. Ceram Soc.* 97 (11): 3434-3441.
5. Luo BC, Wang XH, Wang Y, Li LT (2014) Fabrication, characterization, properties and theoretical analysis of ceramic/PVDF composite flexiblefilms with high dielectric constant and low dielectric loss. *J Mater Chem A* 2:510-519.

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Biography

Xiaohui Wang is a Professor of Department of Materials Science & Engineering at Tsinghua University. She completed her PhD in Physical Chemistry from Jilin University in 1994 , China and her post doctoral work at University of Pennsylvania,USA. Her current research activities include the synthesis and characterization of nano-materials, sintering of nanoceramics and its applications. She has published more than 300 papers in reputed journals.

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