

Supplementary Information

Tailoring the Structural and Electro-Optical Properties of Visible-Light Emitting BaZrO₃ Photo-catalyst: Integrating DFT and Comprehensive Experimental Analysis

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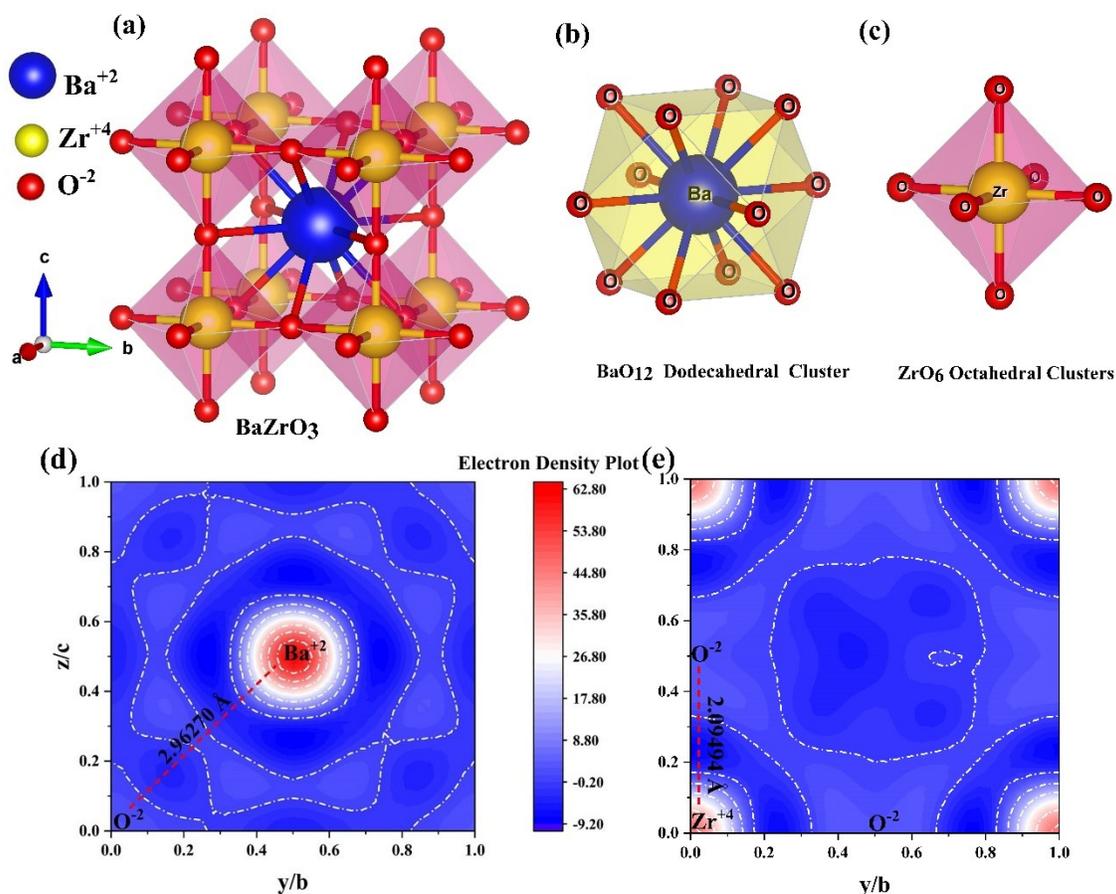


Figure S1(a). Crystallographic representation of BaZrO₃ Nanoparticles, **S1(b)** BaO₁₂ dodecahedral cluster, **S1(c)** ZrO₆ octahedral clusters and **S1(d-e)** Electron density plots of BaZrO₃

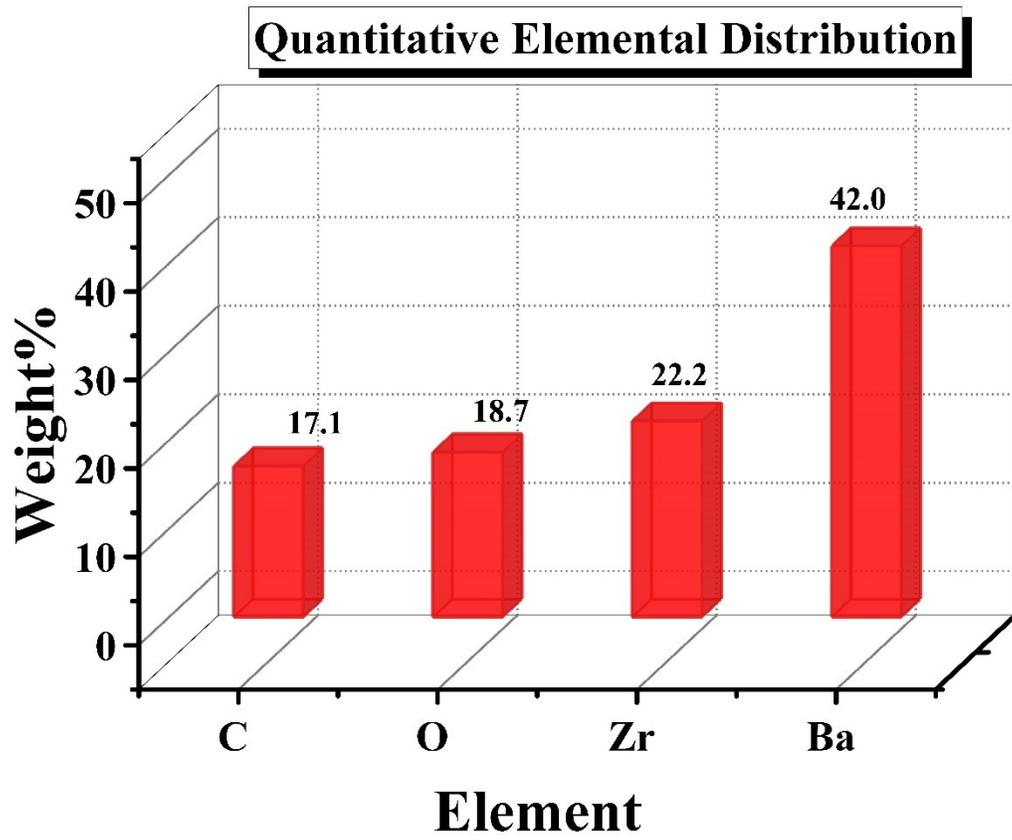


Figure S2. elemental distribution graph of BaZrO₃ nanoparticles.

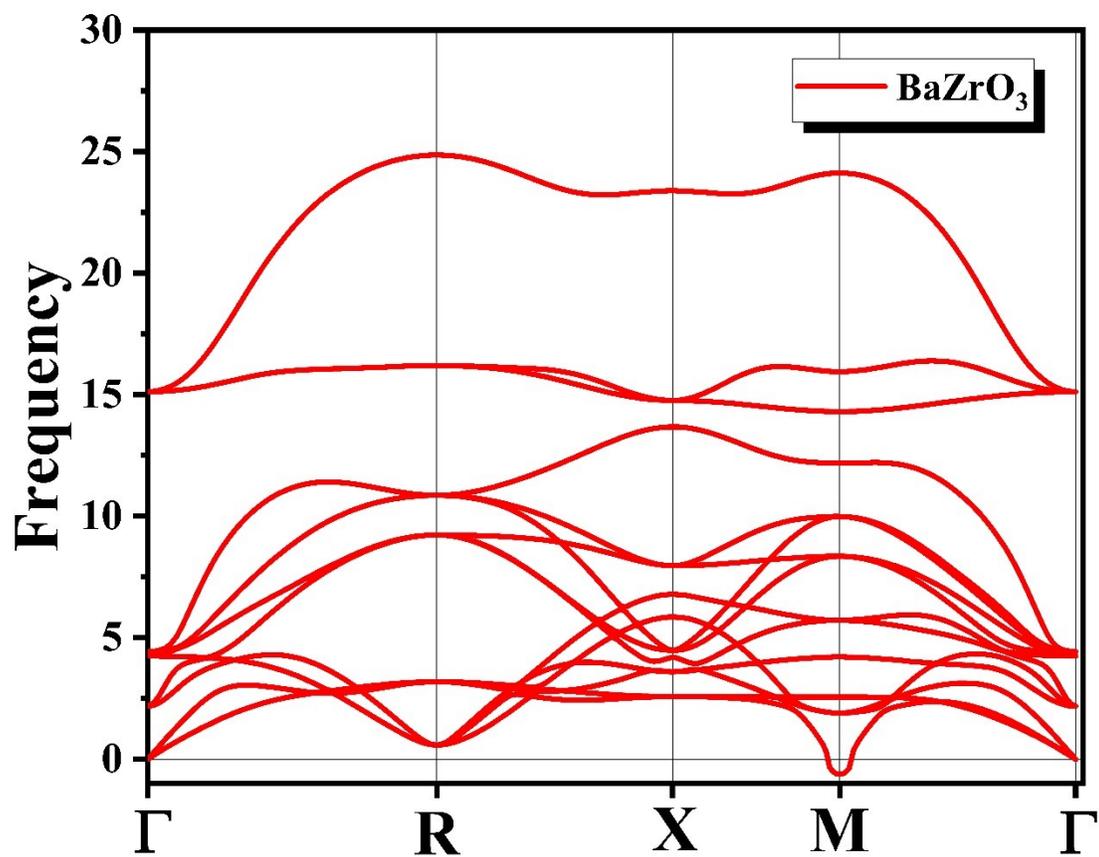


Figure S3. Phonon Spectra of BaZrO₃ nanoparticles.

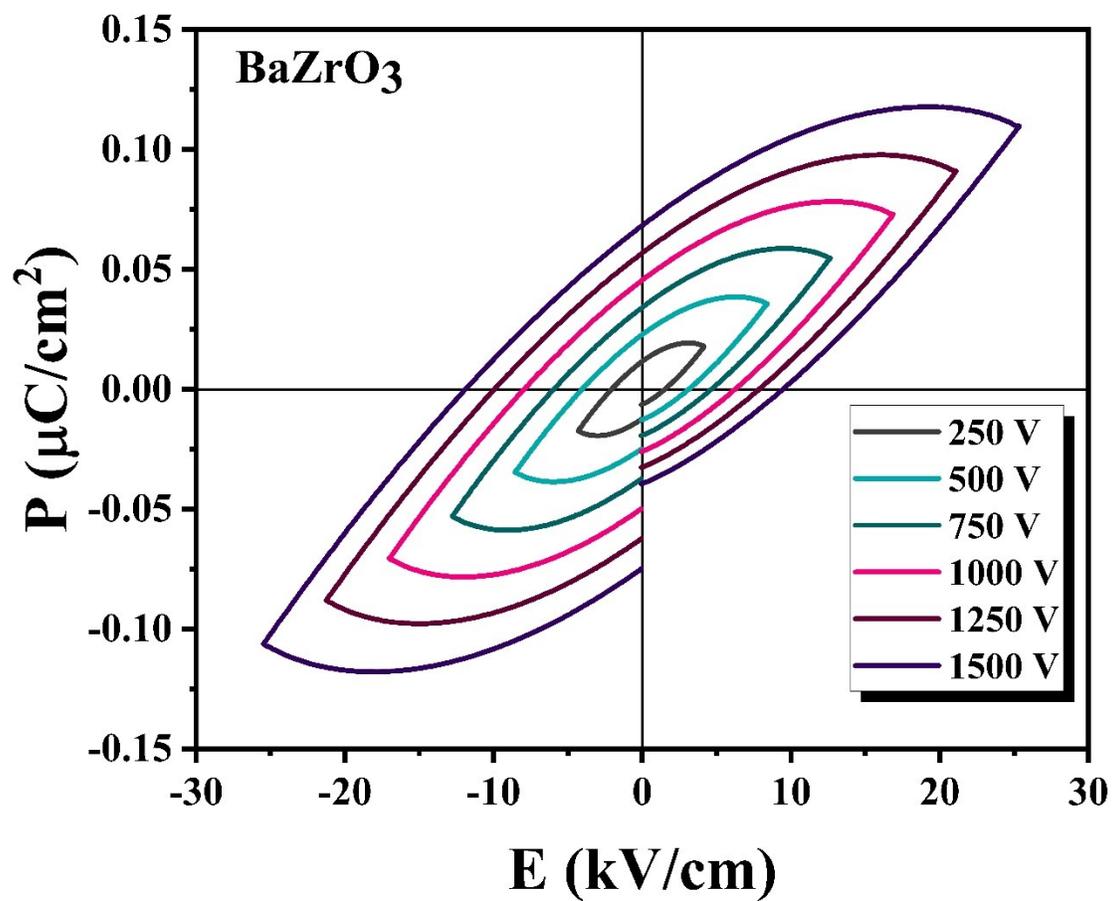


Figure S4. Ferroelectric PE Loop Analysis of BaZrO₃ ceramic.

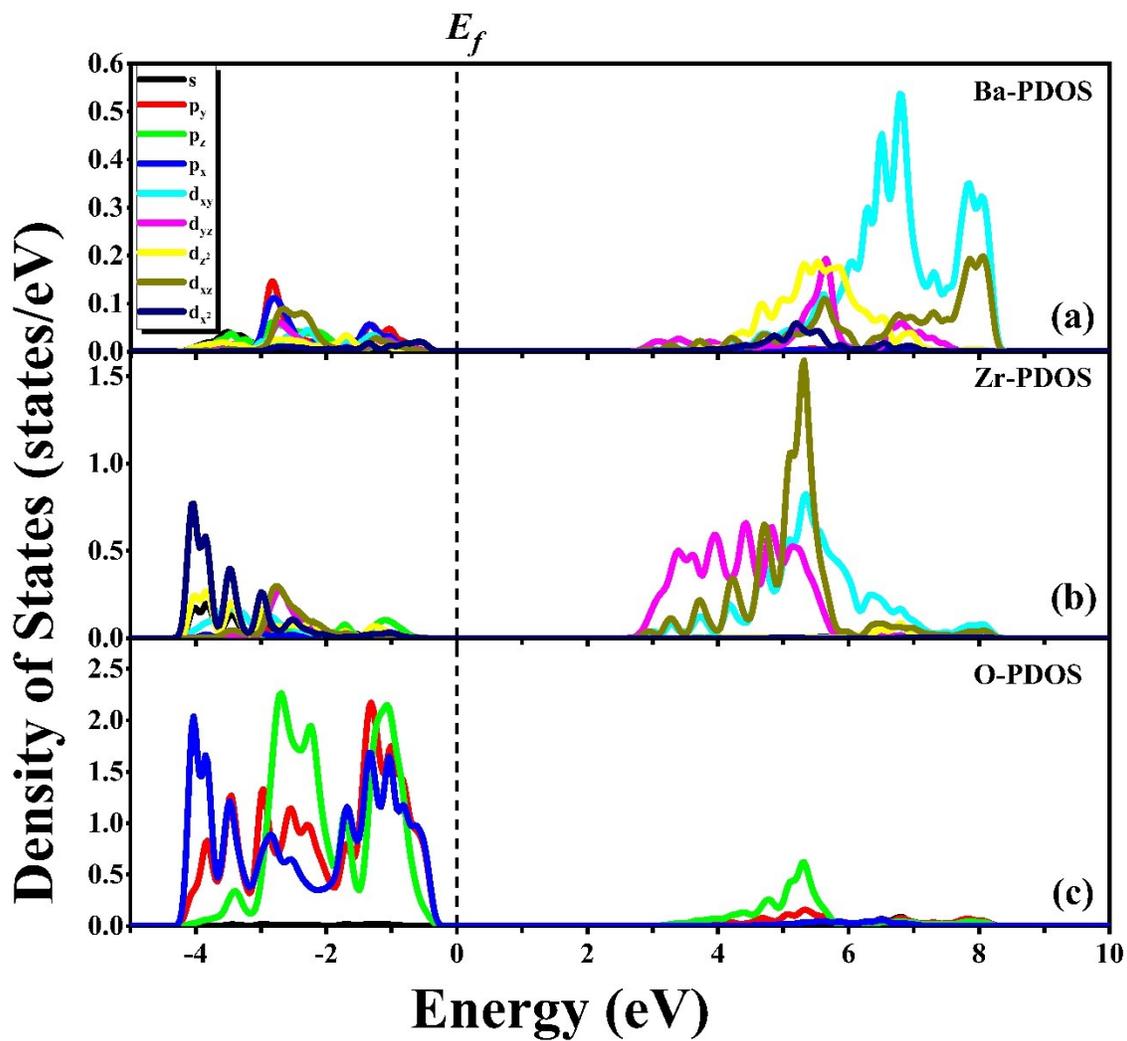


Figure S5. Partial Density of States (PDOS) of BaZrO₃.