Unraveling the synthesis, structure, and properties of zirconia nanocrystals

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Energy and memory storage systems play a vital role in numerous applications, ranging from consumer electronics to renewable energy. Ongoing research aims to enhance the performance and capabilities of these technologies while enabling new applications. One promising avenue for advancement lies in materials with switchable polarization behaviors, such as ferroelectricity, which have the potential to significantly improve developments in this field. Nanomaterials possess unique physical, chemical, and biological properties that differ from their bulk counterparts, making them highly attractive for many applications. However, their properties are often determined by size, shape, and structure, so understanding the relationship between synthesis and structure is crucial for optimizing their properties. In this work, we investigate the formation mechanism of zirconia nanocrystals using a powerful combination of techniques, including X-ray scattering, NMR spectroscopy, quantum chemical calculations, and chromatography.[1, 2] Through these methods, we identified the active precursor species and amorphous intermediate in the reaction mixture and hypothesized an alternative mechanism for precursor decomposition and nanocrystal formation. By using various precursor combinations, we demonstrated several strategies for controlling the kinetics of the reaction and achieving size tuning, which is particularly challenging for group 4 and 5 metal oxides. Furthermore, we conducted a thorough structural characterization of zirconia nanocrystals using pair distribution function analysis, which revealed a distinct local structure distortion in the material. Intriguingly, this distortion induces switchable polarization properties in ZrO_2. Overall, our study sheds new light on the formation and properties of zirconia nanocrystals and opens up new possibilities for the design of novel energy and memory storage systems based on switchable polarization behaviors.

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2. Pokratath, R.; Van Den Eynden, D.; Cooper, S. R.; Mathiesen, J. K.; Waser, V.; Devereux, M.; Billinge, S. J. L.; Meuwly, M.; Jensen, K. M. Ø.; De Roo, J., Mechanistic Insight into the Precursor Chemistry of ZrO_2 and HfO_2 Nanocrystals; towards Size-Tunable Syntheses. *JACS Au*, 2, 4, 827-838, **2022**.