Supplementary Materials: Pair Distribution Function Analysis of ZrO₂ Nanocrystals and Insights in the Formation of ZrO₂-YBa₂Cu₃O₇ Nanocomposites

Hannes Rijckaert ¹, Jonathan De Roo ¹, Matthias Van Zele ¹, Soham Banerjee ², Hannu Huhtinen ³, Petriina Paturi ³, Jan Bennewitz ⁴, Simon J. L. Billinge ^{2,5}, Michael Bäcker ⁶, Klaartje De Buysser ¹ and Isabel Van Driessche ^{1,*}

- ¹ Ghent University, SCRiPTS, Dept. of Chemistry, Krijgslaan 281-S3, 9000 Ghent, Belgium; Hannes.Rijckaert@ugent.be (H.R.); Matthias.VanZele@ugent.be (M.V.Z.); Jonathan.DeRoo@ugent.be (J.D.R.); Klaartje.DeBuysser@ugent.be (K.D.B.)
- ² University of Turku, Wihuri Physical Laboratory, Dept. of Physics and Astronomy, 20014 Turku, Finland; Hannu.Huhtinen@utu.fi (H.H.); Petriina.Paturi@utu.fi (P.P.)
- ³ BASF SE, Advanced Materials & Systems Research, Carl-Bosch-Straße 38, 67056, Ludwigshafen am Rhein, Germany; Jan.Bennewitz@basf.com (J.B.)
- ⁴ Dept of Applied Physics and Applied Mathematics, Columbia University, 1105 S.W. Mudd, New York, NY 10027; sb3519@columbia.edu (S.B.); sb2896@columbia.edu (S.B.)
- ⁵ Deutsche Nanoschicht GmbH, Heisenbergstraße 16, 53359 Rheinbach, Germany; Baecker@d-nano.com (M.B.)
- * Correspondence: Isabel.VanDriessche@ugent.be; Tel.: +32-9263-4433

Refined crystal structure



Figure S1. (left) tetragonal and (right) distorted tetragonal crystal structure for ZrO2 after PDF refinement.

Nuclear Magnetic Resonance analysis of the bisphosphonate stabilized nanocrystals



Figure S2. (A) 1D ¹H spectrum and (B) ³¹P spectrum of ZrO₂ nanocrystals stabilized with bisphosphonate (BP) in MeOD-*d*₄, with (C) a zoom on BP resonances.



Figure S3. Bi-exponential diffusion decay fitting of the bisphosphonate ligand.