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Structure investigation of ultra-small CdSe nanoparticles using the atomic PDF AHMAD S. MASADEH, Dept of Phys, University of Jordan, Amman 11942, Jordan, SIMON J.L. BILLINGE, EMIL S. BOZIN, Dept of Applied Phys and Applied Math., Columbia University, NY, 10027, and Condensed Matr. Dept., BNL., Upton, NY, 11973 USA, JAMES R. MCBRIDE, SANDRA J. ROSENTHAL, Dept of Chem, Vanderbilt University, Nashville, TN 37235, USA — The size-dependent structure of CdSe nanoparticles, with diameter ranging from 1.5 to 3.6 nm, has been studied using the atomic pair distribution function (PDF) method. The samples are prepared by the methods of Peng *et al* [1], with modifications. The structure of the smallest stable size, (~ 1.5 nm), have been found to possess locally distorted wurtzite structure, with no clear evidence of a heavily disordered surface region [2]. The PDF data of the smallest particle show an extra structural peak appears around $r = 3.5$ Å indicates there is structure modification happened in this sample. This peak start appearing the nanoparticles PDF data gradually as nanoparticle size decreases. The structural parameters are reported quantitatively. We measure a size-dependent strain on the Cd-Se bond which reaches 1.0% at the smallest particle size [3]. The size of the well-ordered core extracted directly from the data agrees with the size determined from other methods.
[1] Peng, et al, *JACS.*, 120, 5343-5344 (1998). [2] Gilbert et al, *Science*, 305, 651-654 (2004). [3] Masadeh et al. *PRB* **76**, 115413 (2007).

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