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Study of colloidal quantum dot surfaces using an innovative thin-film positron 2D-ACAR method B. BARBIELLINI, A. BANSIL, Northeastern U., S. W. H. EIJT, H. SCHUT, Delft University of Technology, P. E. MIJNARENDS, Northeastern U. and Delft University of Technology, A. B. DENISON, Lawrence Livermore National Laboratory — Despite a wealth of information, many fundamental questions regarding the nature of the surface of nanosized inorganic particles and its relationship with the electronic structure remain unsolved. We have investigated the electron momentum density (EMD) of colloidal CdSe quantum-dots via depth-resolved positron 2D angular correlation of annihilation (2D-ACAR) spectroscopy at the Delft intense variable-energy positron beam. This method, in combination with first-principles calculations of the EMD, shows that implanted positrons are trapped at the surface of CdSe nanocrystals. They annihilate mostly with the Se electrons and monitor changes in composition and structure of the surface while hardly sensing the ligand molecules. We thus unambiguously confirm [1] the strong surface relaxation predicted by first-principles calculations [2]. Work supported by the USDOE.

[1] S.W.H. Eijt *et al.*, Nature Materials (in press).

[2] A. Puzder, *et al.*, Phys. Rev. Lett. 92, 217401 (2004).

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