Surfaces of nanomaterials for sustainable energy applications: thin-film 2D-ACAR and PALS studies

B. BARBIELLINI, Northeastern University, L. CHAI, Delft U. Tech., W. AL-SAWAI, Northeastern U., S.W.H. EIJT, P.E. MIJNARENDS, H. SCHUT, Y. GAO, A.J. HOUTEPEN, Delft U. Tech., L. RAVELLI, W. EGGER, U. der Bundeswehr Muenchen, M.A. VAN HUIS, Utrecht U., A. BANSIL, Northeastern U. — Positron (e\(^+\)) annihilation spectroscopy is one of only a few techniques to probe the surfaces of nanoparticles. We investigated thin films of PbSe colloidal semiconductor nanocrystals (NCs) in the range 2-10 nm as prospective highly efficient absorbers for solar cells. We compare and contrast our findings with previous studies on CdSe NCs. Evidence obtained from our e\(^+\) lifetime spectroscopy study using the PLEPS spectrometer shows that 90-95% of the implanted positrons are effectively trapped and confined at the surfaces of these NCs. The remaining 5-10% of the e\(^+\) annihilate in the relatively large oleic acid ligands, in fair agreement with the estimated positron stopping power of the PbSe nanoparticle “core” relative to the ligand “shell.” 2D-ACAR measurements on the same set of films using the low-energy e\(^+\) beam POSH showed that the e\(^+\) wavefunction at the surfaces of the PbSe NCs is more localized than for the case of CdSe NCs. Comparison with calculated e\(^+\) - e\(^-\) momentum densities indicates a Pb deficiency at the surfaces of the PbSe NCs, which correlates with e\(^+\) lifetime and the NCs morphology.

\(^1\)Work supported in part by the US Department of Energy.