

Supporting Information

5.2% Efficient PbS Nanocrystal Schottky Solar Cells

*By Claudia Piliago,[†] Loredana Protesescu,[‡] Satria Zulkarnaen Bisri,[†] Maksym V. Kovalenko,[‡]
and Maria Antonietta Loi^{†*}*

[†]Zernike Institute for Advanced Materials, University of Groningen, Nijenborgh 4, Groningen,
9747 AG, The Netherlands

[‡]Department of Chemistry and Applied Biosciences, ETH Zürich, Wolfgang-Pauli-Str. 10,
Zurich, 8093 and EMPA-Swiss Federal Laboratories for Materials Science and Technology,
Überlandstrasse 129, Dübendorf, 8600, Switzerland.

Email: m.a.loi@rug.nl

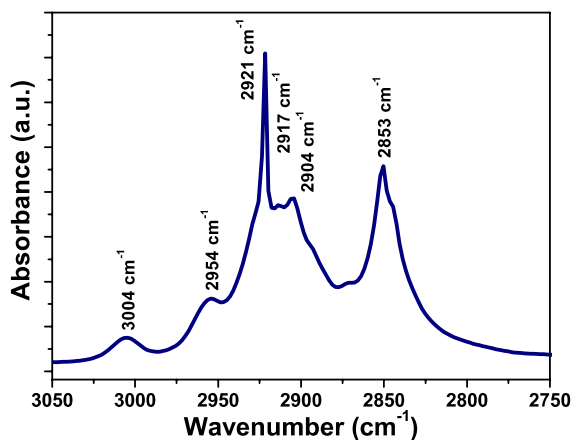


Figure S1. FTIR spectra for *PbS*₃ washing steps: the peaks at 2921 cm⁻¹, 2917 cm⁻¹, 2904 cm⁻¹ and 2853 cm⁻¹ are assigned to antisymmetric and symmetric methylene stretch modes ($\nu_{(as)}\text{CH}_2$, $\nu_{(s)}\text{CH}_2$).

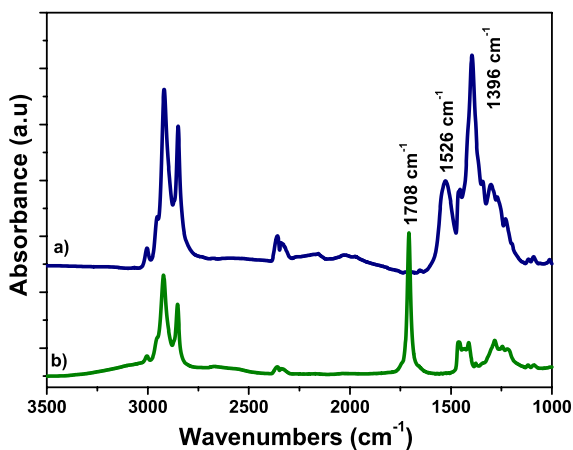


Figure S2: FTIR spectra for a) *PbS*₄ washing steps the wavenumbers separation between $\nu_{as}(\text{COO}^-)$ -1526 cm⁻¹ and $\nu_s(\text{COO}^-)$ -1396 cm⁻¹ is 130 cm⁻¹ and it can be assigned to a bidentate coordination. b) Oleic acid: the peak at 1708 cm⁻¹ corresponds to the C=O stretching of carboxylate in acidic form.

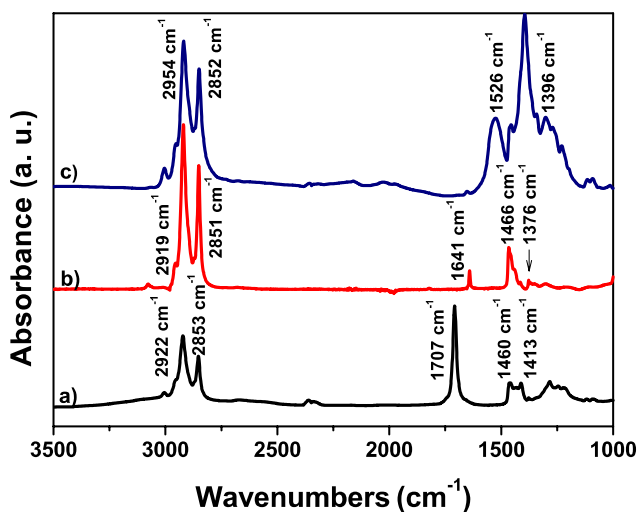


Figure S3. FTIR spectra for *a) oleic acid*: 2922 cm^{-1} $-v_{\text{as}}(\text{C-H in CH}_2 \text{ and CH}_3)$, 2853 cm^{-1} $-v_{\text{s}}(\text{C-H in CH}_2)$, 1707 cm^{-1} $v(\text{C=O})$ -acidic form, 1460 cm^{-1} , 1413 cm^{-1} $-\delta(\text{C-H in CH}_2)$ -bending and scissoring vibration mode, *b) octadecene*: 2919 cm^{-1} $-v_{\text{as}}(\text{C-H in CH}_2 \text{ and CH}_3)$, 2851 cm^{-1} $-v_{\text{s}}(\text{C-H in CH}_2)$, 1641 cm^{-1} $v(\text{C=C})$ -, 1466 cm^{-1} $v(\text{C-H in CH}_2)$ -bending vibrations, 1376 cm^{-1} umbrella type of vibration, *c) PbS 4 washing steps*: 2954 cm^{-1} $-v_{\text{as}}(\text{C-H in CH}_2 \text{ and CH}_3)$, 2852 cm^{-1} $-v_{\text{s}}(\text{C-H in CH}_2)$ $v_{\text{as}}(\text{COO}^-)$ - 1526 cm^{-1} and $v_{\text{s}}(\text{COO}^-)$ - 1396 cm^{-1} .

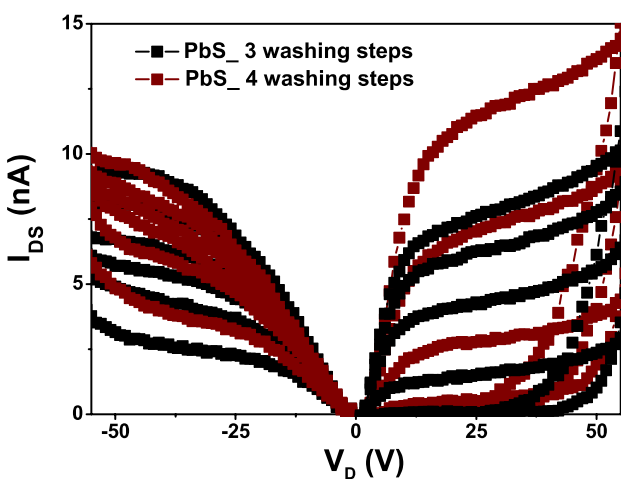


Figure S4 p-channel and n-channel I_D - V_D output characteristics of FETs of PbS colloidal nanocrystal fabricated using solutions with 3 and 4 washing steps. The electron mobilities, extracted from the transfer curves in saturation regimes are: *PbS_3 washing steps* $1.2 \times 10^{-5}\text{ cm}^2/\text{Vs}$ and *PbS_4 washing steps* $2 \times 10^{-5}\text{ cm}^2/\text{Vs}$.

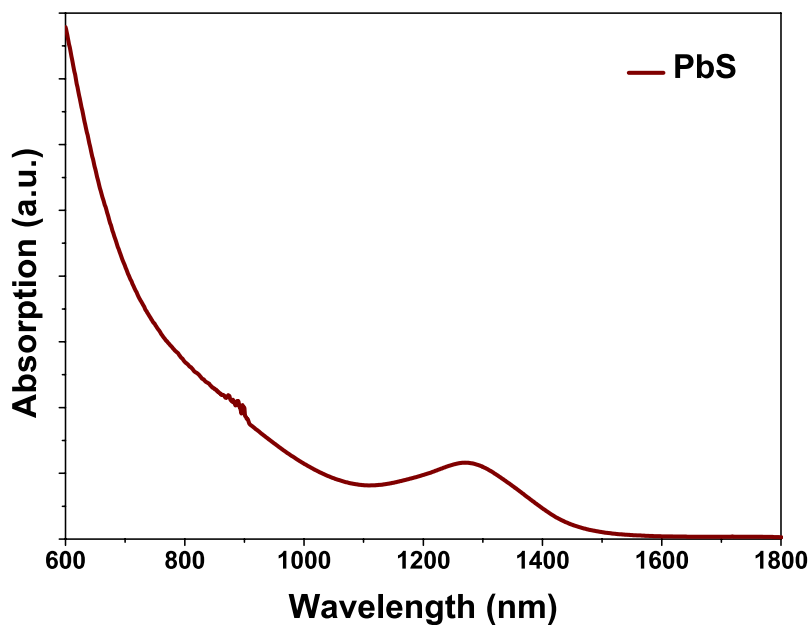


Figure S5 Absorption spectra of OA-capped PbS nanocrystals dispersed in chloroform.

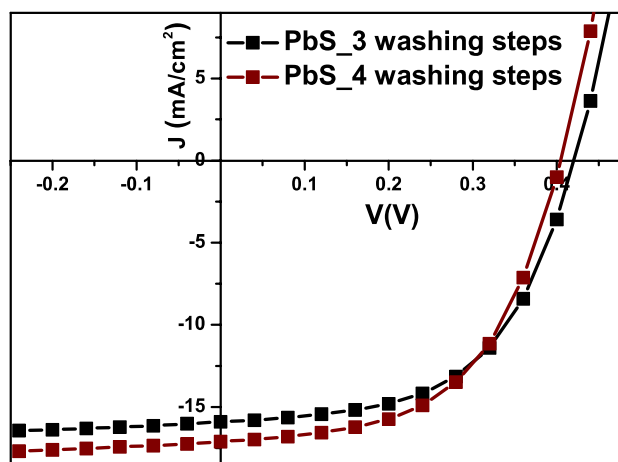


Figure S6 J - V current-voltage characteristics of the devices realized from PbS solutions with 3 and 4 washing steps.

Table 1. Comparison of performance parameters between solar cells fabricated from the solutions of PbS nanocrystal that have been washed three times and four times

	V_{oc} (V)	J_{sc} (mA/cm²)	FF (%)	PCE (%)
PbS_3 washing steps	0.42	-15.9	55	3.7
PbS_4 washing steps	0.4	-17.2	55	3.8