Electronic Supplementary Information (ESI) *for*

Synthesis cost dictates the commercial viability of lead sulfide and perovskite quantum dot photovoltaics

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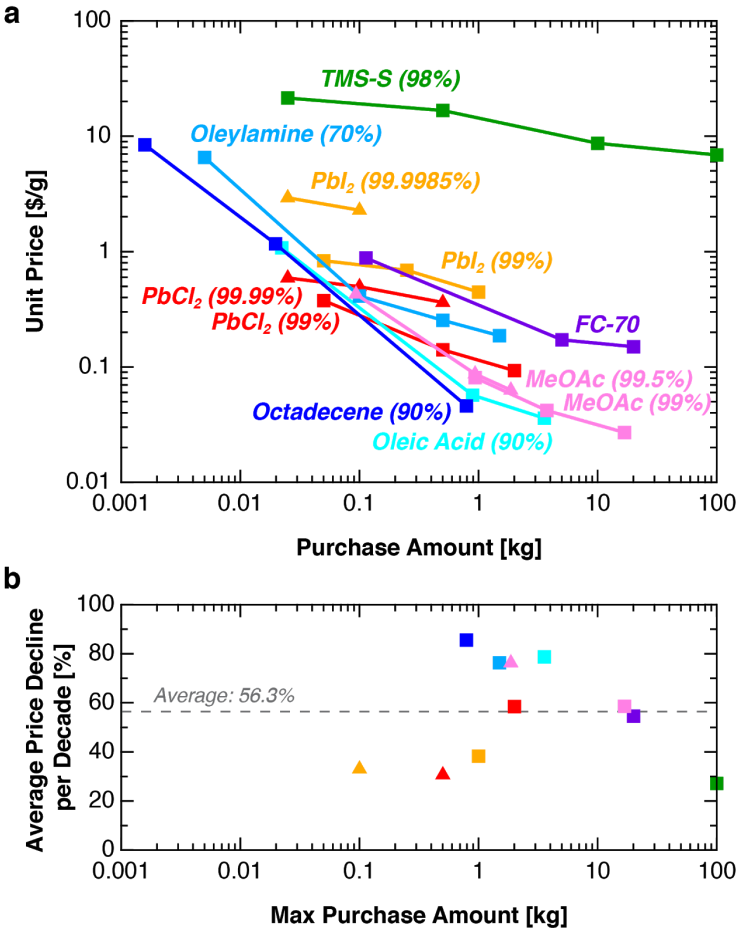

Figure S1: Economies of scale in purchase of raw materials. (a) Quoted price per gram at different purchase volumes for materials from leading commercial suppliers. Price reductions with increasing scale likely arise both from lower supplier profit margins and from lower unit costs with larger batch sizes. (b) Average reduction in price per gram for every 10× increase in purchase volume. The average price reduction across all materials shown is 56.3% per decade.

Table S1: Summary of QD synthesis and ink preparation methods used in cost analysis.

QD Type	Strategy	Precursor 1	Precursor 2	Reference	Materials	Crashout	Reported Yield
PbS	Hot injection	PbO	TMS-S	Pan 2013	0.9g PbO (99%), 3mL OA (tech grade 90%), 6mL ODE (tech grade 90%), 30mL ODE, 20mL FC-70, 360µL TMS-S (95%), 20mL ODE, 20mL FC-70	Assumed Chang 2013 recipe	40-42mg/min = 2.4-2.5 g/h
				Yarema 2017	18g PbO, 70mL OA, 730mL ODE, 8.4mL TMS-S, 400mL ODE	Mix 1.2L growth solution with 0.6L hexane and 2.2L acetone and centrifuge, Redisperse in 0.75L hexane and precipitate with 0.75L acetone (3x)	17.2g PbS
			Thiourea	Hendricks 2015	3mmol alkylamine in 2.5mL toluene, 3mmol alkyl or aryl isothiocyanate in 2.5mL toluene	6 total crashouts from toluene using methyl acetate: Growth solution + 40mL toluene + 120mL methyl acetate	100% yield
					10g PbO (99.999+%), 20mL ACN (99.5%), 0.7mL TFA (99%), 6.2mL TFAA (≥99%), 25.437g OA (99%), 180mL IPA (≥99.7%), 10.246g Et3N (≥99%), 900mL MeOH		31.1–32.8g Pb(oleate)2 (90–95% yield) through lead trifluoroacetate route
					8.812g Pb(oleate)2, 105.5g (147.5mL) 1-octene (99%), 1.742g N,N'-diphenylthiourea (98%), 5mL diglyme (99.5% anhydrous)		2.67g (79.5%) yield of (PbS)(Pb(oleate)2) 0.26
		PbAc	TMS-S	Chang 2013	11.38g PbAc, 21mL OA, 300mL ODE, 3.15 mL TMS-S, 150mL ODE	1 crashout after synthesis: 15:18:5 growth solution:acetone:butanol, 5:1 supernatant:acetone, Redisperse 1:1 in hexane 2 crashouts before device fab: 1:0.2:0.8:1.5 crude:butanol:ethanol:acetone, Redisperse 1:1 in hexane	3.7g PbS (estimated)
		PbCl2	Sulfur	Moreels 2011	0.024g Sulfur (99.999%), 2.25mL OLA (80-90%), 0.834g PbCl2 (99.999%), 7.5mL OLA, 170µL TOP (97%), 10mL toluene (quenching), 15mL EtOH (quenching)	Assumed Chang 2013 recipe	20–30% yield with TOP
	Heat-up	PbCl2	TMS-S	Zhang 2014	83.4g PbCl2 (99.999%), 600mL OLA (70% tech grade), 21mL TMS-S (synthesis grade), 20mL OLA	Assumed Chang 2013 recipe	47.07g for large-scale synthesis (~50% yield for both Pb and S precursors at small scale, slightly lower at large scale)
			TAA	Huang 2017	3 mmol PbCl2 (99.99%), 10mL OLA (80–90%), 1 mmol thioacetamide (TAA, ≥99%), 2mL OLA	Assumed Chang 2013 recipe	40x quantities for large-scale synthesis: 18g output (80% sulfur conversion)
CsPbI3	Hot injection	Cs2CO3	PbI2	Sanehira 2017	Cs-oleate solution in ODE: 0.407g Cs2CO3 (SA, 99.9%), 1.25mL OA (SA, 90%), 20mL ODE (SA, 90%) CsPbI3 QDs: 0.5g PbI2 (Alfa Aesar, 99.9985%), 25mL ODE, 2.5mL OA, 2.5mL OAm (SA, 70%), 2mL Cs-oleate solution (see above)	1st crashout: 35mL methyl acetate (MeOAc, SA, 99.5% anhydrous), 15mL QD reaction liquor, 5mL hexane 2nd crashout: 6.5mL MeOAc, 15mL hexane Store in dark at 4°C for ≥24 hours to precipitate excess Cs-oleate and Pb-oleate Remove solid precipitates by centrifugation before use	
PbS Ink	Biphasic exchange	PbI2	PbBr2	Liu 2016	5mL of 10mg/mL PbS QD in octane, 230.5 mg PbI2 + 36.7mg PbBr2 + 15.4mg NH4Ac in 5mL DMF, Volume for octane rinse and toluene crashout unreported (5:2.7 DMF: toluene reported by Aqoma 2018), 0.25mL butylamine (resuspension)		
			N/A	Aqoma 2017	5mL of 15 mg/mL PbS QD in octane, 691mg PbI2 (Alfa Aesar, 99.99%) in 5mL DMF, Volume for octane rinse unreported, 0.5 mL butylamine (resuspension)		

Table S2: Cost breakdown for all QD synthesis and ink preparation methods analyzed.

		QD Synthesis								Ink Preparation	
	QD Type	**PbS**							**$CsPbI_3$**	**PbS**	
	Precursor 1	$PbCl_2$	$PbCl_2$	PbO	PbAc	PbO	PbO	$PbCl_2$	Cs_2CO_3	PbI_2	PbI_2
	Precursor 2	TAA	TMS-S	TMS-S	TMS-S	Thiourea	TMS-S	Sulfur	PbI_2		$PbBr_2$
	Method	Heat up	Heat up	Hot injection	Hot injection	Hot injection	Flow	Hot injection	Hot injection	Phase transfer	Phase transfer
	Reference	Huang 2017	Zhang 2014	Yarema 2017	Chang 2013	Hendricks 2015	Pan 2013	Moreels 2011	Sanehira 2017	Aqoma 2017	Liu 2016
$/g	**TOTAL**	**10.6**	**10.7**	**17.4**	**26.6**	**32.3**	**35.7**	**59.2**	**72.7**	**6.3**	**8.7**
	Sum of Medians	*7.6*	*7.8*	*14.5*	*23.6*	*29.2*	*32.7*	*56.1*	*69.0*	*5.2*	*7.7*
	Materials	3.2	4.7	5.3	9.3	8.7	13.7	21.5	17.5	3.7	5.4
	Labor	3.5	2.0	7.5	11.8	17.5	15.6	29.0	44.7	1.5	2.2
	CapEx	0.1	0.0	0.1	0.2	0.3	0.3	0.5	0.7	0.0	0.1
	OpEx	0.0	0.0	0.0	0.1	0.1	0.1	0.1	0.2	0.0	0.0
	Yield Loss	0.9	0.9	1.5	2.3	2.7	3.1	5.1	5.9	0.0	0.0
$/m² *(500nm film)*	**TOTAL**	**28.6**	**29.0**	**47.2**	**72.0**	**87.4**	**96.7**	**160.1**	**139.7**	**17.0**	**23.6**
	Sum of Medians	*20.6*	*21.0*	*39.2*	*63.7*	*78.9*	*88.6*	*151.9*	*132.6*	*14.1*	*20.8*
	Materials	8.7	12.8	14.5	25.1	23.4	37.0	58.1	33.6	10.0	14.7
	Labor	9.4	5.5	20.4	31.8	47.3	42.2	78.4	85.9	4.0	6.0
	CapEx	0.2	0.1	0.3	0.5	0.8	0.7	1.3	1.4	0.1	0.1
	OpEx	0.0	0.0	0.1	0.1	0.2	0.2	0.3	0.4	0.0	0.0
	Yield Loss	2.4	2.6	4.0	6.1	7.2	8.4	13.8	11.4	0.0	0.0
$/W *(19% PCE)*	**TOTAL**	**0.15**	**0.15**	**0.25**	**0.38**	**0.46**	**0.51**	**0.84**	**0.74**	**0.09**	**0.12**
	Sum of Medians	*0.11*	*0.11*	*0.21*	*0.34*	*0.42*	*0.47*	*0.80*	*0.70*	*0.07*	*0.11*
	Materials	0.05	0.07	0.08	0.13	0.12	0.19	0.31	0.18	0.05	0.08
	Labor	0.05	0.03	0.11	0.17	0.25	0.22	0.41	0.45	0.02	0.03
	CapEx	0.00	0.00	0.00	0.00	0.00	0.00	0.01	0.01	0.00	0.00
	OpEx	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
	Yield Loss	0.01	0.01	0.02	0.03	0.04	0.04	0.07	0.06	0.00	0.00

Table S3: Cost breakdown by process step for QD synthesis and ink preparation methods.

		QD Synthesis								Ink Preparation	
	QD Type	**PbS**							**$CsPbI_3$**	**PbS**	
	Precursor 1	$PbCl_2$	$PbCl_2$	PbO	PbAc	PbO	PbO	$PbCl_2$	Cs_2CO_3	PbI_2	PbI_2
	Precursor 2	TAA	TMS-S	TMS-S	TMS-S	Thiourea	TMS-S	Sulfur	PbI_2		$PbBr_2$
	Method	Heat up	Heat up	Hot injection	Hot injection	Hot injection	Flow	Hot injection	Hot injection	Phase transfer	Phase transfer
	Reference	Huang 2017	Zhang 2014	Yarema 2017	Chang 2013	Hendricks 2015	Pan 2013	Moreels 2011	Sanehira 2017	Aqoma 2017	Liu 2016
Synthesis	**SUM [$/g]**	**2.1206**	**4.3971**	**5.8039**	**9.2961**	**11.9388**	**14.7553**	**19.6929**	**21.5933**	**5.2038**	**7.6957**
	Materials	0.9829	3.7377	3.3072	5.5100	6.1716	9.6559	11.0275	6.8348	3.6835	5.4180
	Capex	0.0276	0.0159	0.0604	0.0929	0.1395	0.1243	0.2093	0.3554	0.0369	0.0547
	Labor	1.1029	0.6394	2.4206	3.6693	5.5914	4.9428	8.4015	14.3110	1.4739	2.2088
	Opex	0.0072	0.0042	0.0157	0.0240	0.0363	0.0324	0.0546	0.0920	0.0095	0.0141
	Yield loss	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
Crashout	**SUM [$/g]**	**4.2057**	**2.6074**	**5.9714**	**9.7145**	**10.6651**	**12.0918**	**23.6665**	**30.7454**		
	Materials	2.1726	0.9930	2.0050	3.6590	2.2526	3.9025	10.0264	10.2913		
	Capex	0.0276	0.0161	0.0606	0.0923	0.1384	0.1235	0.2098	0.3543		
	Labor	1.1079	0.6455	2.4113	3.6721	5.5658	4.9119	8.2754	14.0931		
	Opex	0.0072	0.0042	0.0157	0.0240	0.0359	0.0321	0.0542	0.0918		
	Yield loss	0.8903	0.9485	1.4787	2.2671	2.6724	3.1219	5.1007	5.9148		
Cleaning	**SUM [$/g]**	**1.1267**	**0.6466**	**2.4530**	**3.7978**	**5.7799**	**5.1273**	**8.8535**	**14.5769**		
	Materials	0.0263	0.0117	0.0420	0.1121	0.2318	0.1436	0.3629	0.3384		
	Capex	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000		
	Labor	1.1004	0.6349	2.4110	3.6858	5.5481	4.9837	8.4906	14.2385		
	Opex	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000		
	Yield loss	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000		
TOTAL [$/g]		**7.5**	**7.7**	**14.2**	**22.8**	**28.4**	**32.0**	**52.2**	**66.9**	**5.2**	**7.7**

Table S4: Cost breakdown for roll-to-roll manufacturing of QD and perovskite PV modules.

	Absorber	$MAPbI_3$	PbS QD	$CsPbI_3$ QD
$/m²	**TOTAL**	**128.4**	**178.6**	**306.6**
	Sum of Medians	*111.1*	*162.6*	*290.7*
	Materials	64.5	111.2	225.4
	Labor	4.5	4.4	4.4
	CapEx	22.0	21.8	21.8
	OpEx	12.1	11.8	11.8
	Yield Loss	8.1	13.3	27.3
$/W *(19% PCE)*	**TOTAL**	**0.68**	**0.94**	**1.61**
	Sum of Medians	*0.59*	*0.86*	*1.53*
	Materials	0.34	0.59	1.19
	Labor	0.02	0.02	0.02
	CapEx	0.12	0.12	0.12
	OpEx	0.06	0.06	0.06
	Yield Loss	0.04	0.07	0.14