

Supporting Information

Roadmap and roadblocks for the tunability of metal halide perovskites for multi-junction solar cell technology

E. L. Unger^{a,b*}, L. Kegelmann^b, K. Suchan^a, D. Sörell^a, L. Korte^b and S. Albrecht^c

I. Experimental data sets from Master thesis of D. Sörell, Lund University, 2015

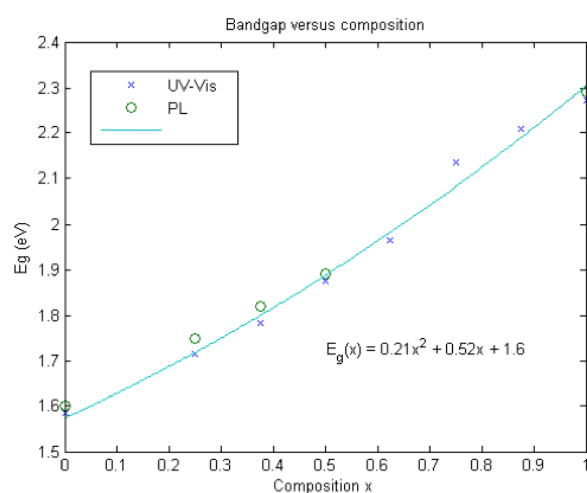


Figure S1a: Experimental data from the master thesis of David Sörell, published at Lund University in 2015 showing the dependence of the bandgap on composition x in $\text{MAPb}(\text{Br}_x\text{I}_{1-x})_3$.

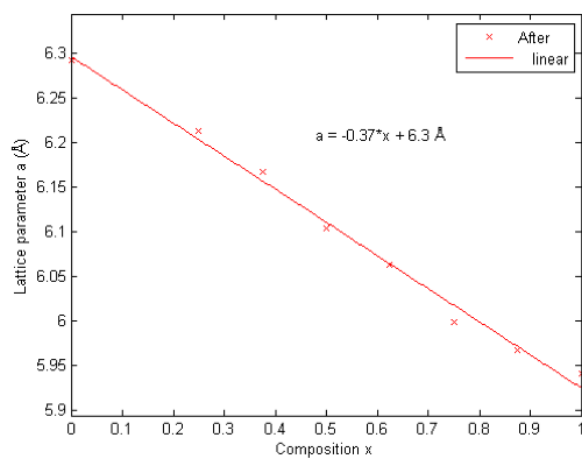


Figure S1b: Experimental data from the master thesis of David Sörell, published at Lund University in 2015 showing the dependence of the pseudocubic lattice parameter a_0 on composition x in $\text{MAPb}(\text{Br}_x\text{I}_{1-x})_3$.

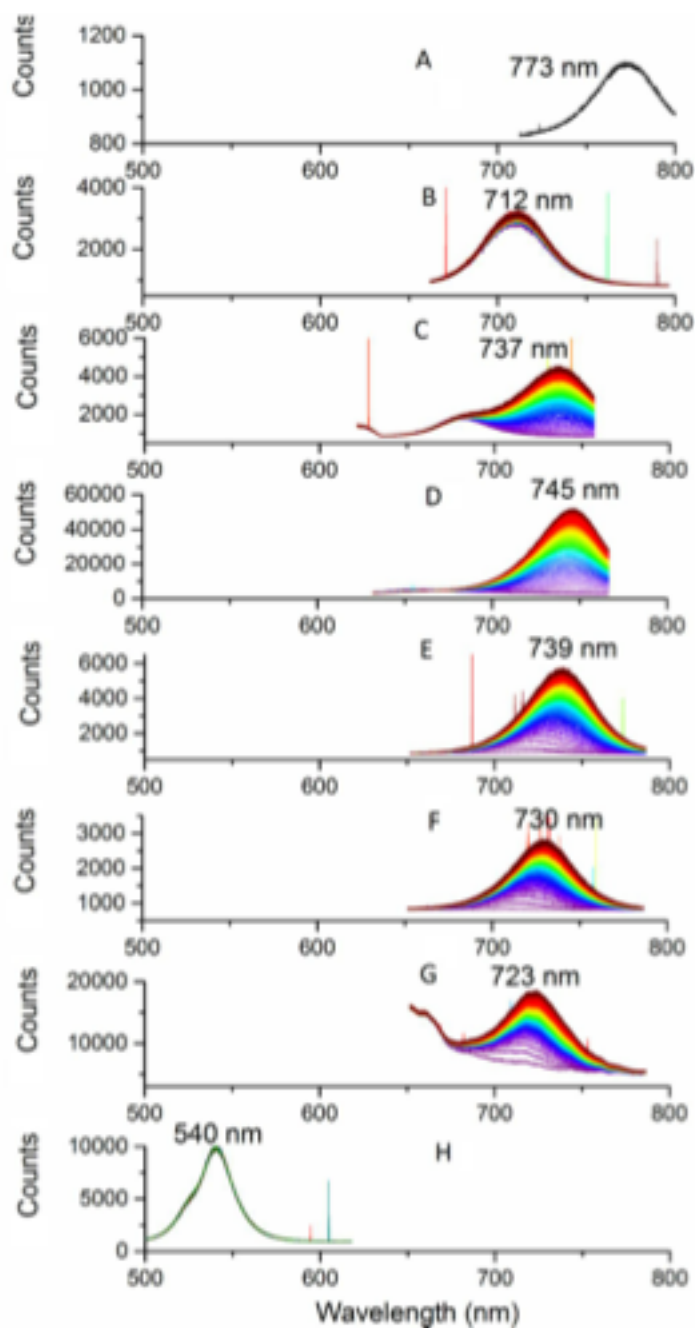


Figure S1c: Experimental data from the master thesis of David Sörell, published at Lund University in 2015 showing the photo-induced shift in the PL spectra for various different compositions of x in $\text{MAPb}(\text{Br}_x\text{I}_{1-x})_3$.

II. Comments on experimental data sets from different literature sources utilized in the comparisons made here.

Short	Figure 1 & 4	Figure 2	Figure 3	© Copyright
Kulbak2015 Ref [22] Kulbak, M. et al. <i>J. Phys. Chem. Lett.</i> 2015.	Device data as table insets shown in Fig.3 used for the comparisons of device performance metrics.			Adapted from Ref [22] published under an ACS Author Choice Licence
Noh2013 Ref [9]	Fig. 4 give PV data as function of composition. Data was digitalized to extract values for band gap, Jsc and Voc.	Fig. 3c shows plots of band gap as function of composition and Figure 2 gives pseudo-cubic lattice parameter as function of composition		Reprinted with permission from references [9]. Copyright 2013 American Chemical Society.
Eperon2014 Ref [14]	Device data shown in Fig 4 was included in comparison	Fig. 2 e displays band gap as function of pseudo-cubic lattice parameter. Band gap estimated from absorption onset		Adapted from ref [14]. Published by The Royal Society of Chemistry (RSC)
Eperon2016 Ref [18]	Device performance data summarized in Table 1.	Band gap vs a_0 determined from Fig. 1 and a_0 was derived from additional data in SI		From Ref [18]. Reprinted with permission from AAAS Copyright 2016.
Beal2016 Ref [17]	Device performance metrics stated in the descriptive text of the article	Band gap energy and pseudo-cubic lattice parameter extracted from Fig. 2 a) by digitalization		Adapted with permission from Ref [17]. Copyright 2016 American Chemical Society
Sutton2016 Ref [16]	Device data for champion cell of CsPbBrI ₂ given in Fig. 3 as table inset		Photoluminescence as a function of composition derived from Fig. 1 c. Data was digitalized	Adapted from ref [16]. Copyright 2016, published by WILEY-VCH Verlag GmbH & Co. KGaA, Weinheim.
Jacobsson2016 Ref [12]	Data for band gaps summarized in Table 1 and Device performance summarized in Table 4 used for this comparison	Data for band gaps summarized in Table 1 and pseudo-cubic lattice parameter derived from unit cell volume compared in Table 2	Values for initial and PL after light soaking were summarized in Table 3 and the supporting information.	Adapted from Ref [12] with permission of The Royal Society of Chemistry (RSC)
McMeekin2016 Ref [35]		Absorption and pseudo-cubic lattice parameter available in supporting information of article		From Ref [35]. Reprinted with permission from AAAS
Heo2014	Device performance			Adapted from ref

Ref [23]	data taken from Table 2 in this manuscript			[23]. Copyright 2016, published by WILEY-VCH Verlag GmbH & Co. KGaA, Weinheim.
Wu2016 Ref [24]	Device performance data taken from Table 1 in the manuscript			Adapted from Ref. [24] with permission of The Royal Society of Chemistry
Forgacs2016 Ref [25]	Data for efficiency values as table inset in Fig. 2 c and f. Band gap estimated from EQE onset in Fig. 2 b and e.			Adapted from ref [25]. Copyright 2016, published by WILEY-VCH Verlag GmbH & Co. KGaA, Weinheim.
Saliba2016 Ref [3]	Device performance data given in article	Band gap as function of lattice constant derived from data sets in article and supporting information.		Adapted from Ref [3] published under a Creative Commons Attribution Non-Commercial 3.0 Unported Licence by The Royal Society of Chemistry (RSC)
Saliba2016 Science Ref [4]	Device performance and band gap of Rb incorporated sample discussed in text.			From Ref [4]. Adapted with permission from AAAS.
Hao2014 Ref [26]	Table 1 provides band gap and device performance metrics	Table 1 also provides pseudo cubic lattice parameters	No information about photostability	Adapted with permission from Macmillan Publisher Ltd: Nature Photonics from Ref [26]. Copyright 2014
Zhao2016 Ref [19]	Data for device performance metrics and band gap available.			Adapted from ref [19]. Copyright 2016, published by WILEY-VCH Verlag GmbH & Co. KGaA, Weinheim.
Zhao2017 Ref [21]	Value for record performance low band gap device included.			Reprinted by permission from Macmillan Publishers Ltd: Nature Energy, copyright 2017
Yang2016 Ref [20]	Device performance metrics as a function of band gap available in the supporting information.			Adapted with permission from ref [20]. Copyright 2016 American Chemical Society.
Mancini2015 Ref [45]		Band gap and pseudo-cubic lattice parameter as		Adapted with permission from Ref [45]. Copyright

		function of composition plotted in Fig.2 and Fig.4. Possibly, higher Sn-content materials have an artificially low band gap as materials may become metallic upon oxidation.		2016 American Chemical Society.
Patrini2016 Ref [46]		Table 1 summarizes data of band gap as function of lattice parameter		Adapted with permission from Ref [46]. Copyright 2016 American Chemical Society.
Fedeli2015 Ref [9]		Band gap as function of composition shown in Figure 3 and lattice parameter as function of composition in Fig. 1 b		Reprinted with permission from references [10]. Copyright 2015 American Chemical Society.
Hoke2015 Ref [11]		Band gap as function of lattice spacing from SI data	Initial and PL after light soaking $\text{MAPb}(\text{Br}_x\text{I}_{1-x})_3$ and $\text{FAPb}(\text{Br}_x\text{I}_{1-x})_3$ shown in main article and supporting information	Reference [11] – Published by The Royal Society of Chemistry 2015.
Rehman2016 Ref [55]			Photo-induced PL peak changes available from Fig. 4 for different compositions	