

Electronic Supplementary Information

Dicyanobenzene Passivated Perovskite Solar Cells with Enhanced Efficiency and Stability

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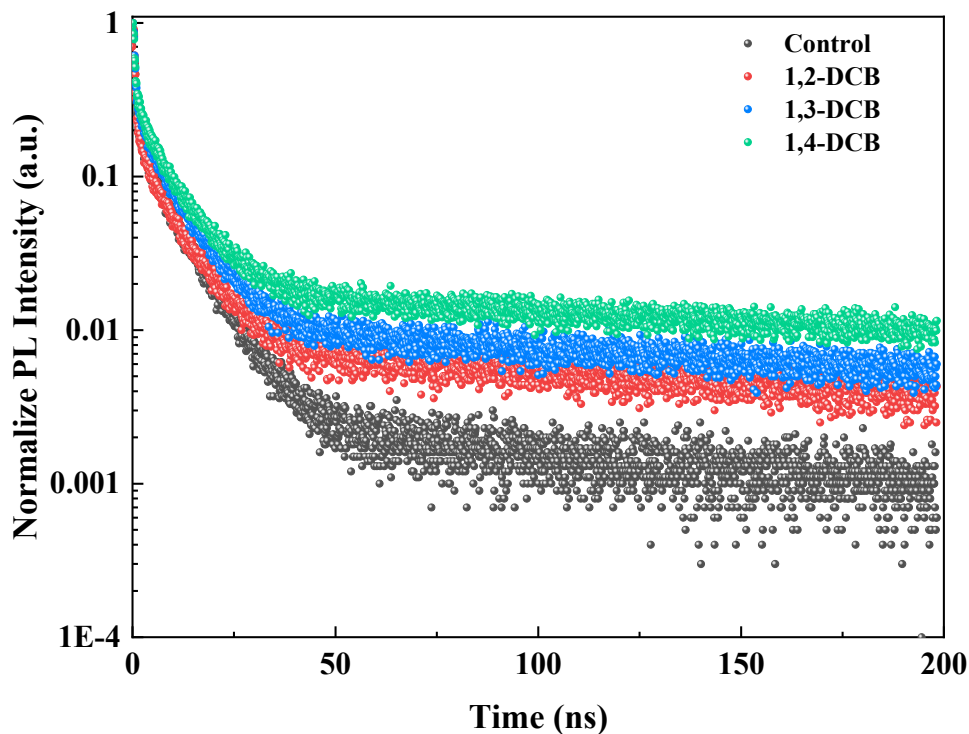


Figure S1. Time-resolved photoluminescence (TRPL) spectra of perovskite films without (control) and with DCB passivation

Table S1. Energies of DCB isomers, PbI_2 , and the 1,2-DCB: PbI_2 , 1,3-DCB: PbI_2 , and 1,4-DCB: PbI_2 complexes, along with the binding energies (E_b 's) of these complexes obtained by energy minimization using the Universal Force Field (UFF) and Merck Molecular Force Field 94 static (MMFF94s) as molecular mechanic functions via Avogadro (version 1.2.0) on the optimized structures of compounds from Gaussian 16 (B3LYP/6-31G(d) basis set).

	Energy of DCB (E_{DCB} ; kJ mol^{-1})	Energy of PbI_2 (E_{PbI_2} ; kJ mol^{-1})	Energy of DCB: PbI_2 ($E_{\text{DCB:PbI}_2}$; kJ mol^{-1})	Binding Energy ($E_b = E_{\text{DCB}} + E_{\text{PbI}_2} - E_{\text{DCB:PbI}_2}$; kJ mol^{-1})
1,4-DCB	186.911	5.05342×10^{-11}	45.6498	141.2612
1,3-DCB	155.374	5.05342×10^{-11}	39.4239	115.9501
1,2-DCB	115.935	5.05342×10^{-11}	45.918	70.017

Table S2. Photovoltaic performance parameters of PSCs passivated with 1,2-DCB solutions with different concentrations.

1,2-DCB conc.	J_{sc} (mA cm ⁻²)		V_{oc} (V)		FF		PCE (%)	
	Best	Average	Best	Average	Best	Average	Best	Average
w/o	21.28	21.20	1.07	1.05	0.80	0.77	18.33	17.59
1 mg/ml	23.41	21.89	1.07	1.06	0.78	0.75	18.86	18.21
2 mg/ml	22.06	21.89	1.08	1.07	0.81	0.80	19.24	18.44
4 mg/ml	21.65	22.90	1.08	1.04	0.81	0.75	19.12	18.15

Table S3. Photovoltaic performance parameters of PSCs passivated with 1,3-DCB solutions with different concentrations.

1,3-DCB conc.	J_{sc} (mA cm ⁻²)		V_{oc} (V)		FF		PCE (%)	
	Best	Average	Best	Average	Best	Average	Best	Average
w/o	21.23	20.37	1.06	1.06	0.80	0.77	18.12	17.44
1 mg/ml	22.34	21.73	1.07	1.06	0.80	0.79	19.14	18.61
2 mg/ml	22.80	22.23	1.09	1.08	0.83	0.82	21.07	19.87
4 mg/ml	22.23	22.18	1.07	1.07	0.83	0.80	20.02	19.08

Table S4. Photovoltaic performance parameters of PSCs passivated with 1,4-DCB solutions with different concentrations.

1,4-DCB conc.	J_{sc} (mA cm ⁻²)		V_{oc} (V)		FF		PCE (%)	
	Best	Average	Best	Average	Best	Average	Best	Average
w/o	21.89	21.08	1.07	1.05	0.77	0.75	18.25	17.60
1 mg/ml	21.42	21.01	1.08	1.06	0.82	0.80	19.49	18.35
2 mg/ml	23.18	22.07	1.09	1.08	0.82	0.81	20.28	19.56
4 mg/ml	22.30	22.21	1.08	1.06	0.82	0.80	20.10	18.91

References

1. D. Yang, R. Yang, X. Ren, X. Zhu, Z. Yang, C. Li and S. F. Liu, *Adv. Mater.*, 2016, **28**, 5206–5213.