

Deuterium-Induced Hydrogen Bond Strengthening: A Novel Strategy for High Stability in Perovskites

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1. Characterization of the D_x MAPbBr₃ deuterium element

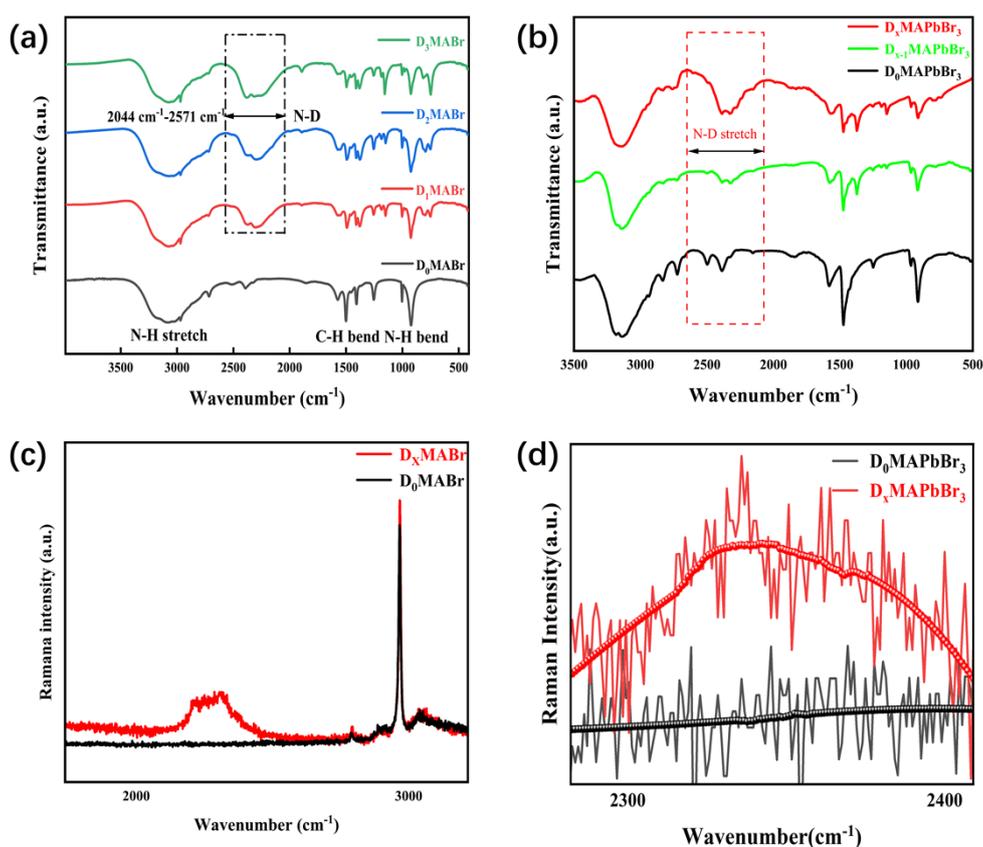


Fig. S1 Fourier Transform Infrared (FTIR) and Raman spectra of non-deuterated MABr and MAPbBr₃ versus deuterated MABr and MAPbBr₃.

2. Stability properties of $D_x\text{MAPbBr}_3$ SC

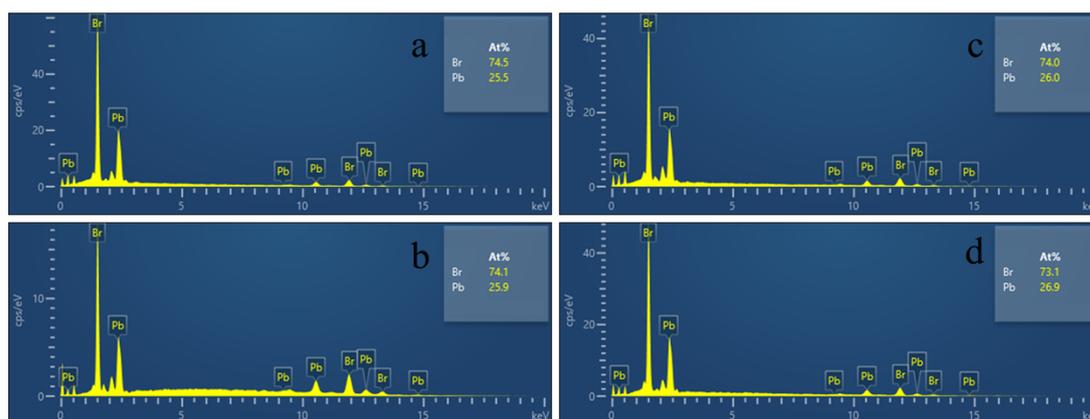


Fig. S2 a and b are unaged $D_x\text{MAPbBr}_3$ SC and $D_0\text{MAPbBr}_3$ SC, respectively, c and d are $D_x\text{MAPbBr}_3$ SC and $D_0\text{MAPbBr}_3$ SC, exposed to air for 60 days, respectively.

3. Assignments of Raman bands of $\text{CH}_3\text{NH}_3\text{PbBr}_3$

No.	Wavenumber / cm^{-1}	Assignments	Orthorhombic	Tetragonal I	Tetragonal II	Cubic
v ₁	328/296	$\text{CH}_3\text{NH}_3^+-\text{PbBr}_3^-$ cage vibration	328/296	325	326	326
v ₂	916	CH_3 rocking and NH_3^+ rocking	916	918	917	916
v ₃	971	C-N ⁺ stretching	971	973	971	969
v ₄	1259	CH_3 rocking and NH_3^+ rocking	1259	1254	1253	---
v ₅	1421	CH_3 symmetric deformation	1421	1424	1423	---
v ₆	1456	CH_3 degenerate deformation	1456	1458	---	---
v ₇	1461	CH_3 degenerate deformation	1461	---	---	---
v ₈	1472	NH_3^+ symmetric deformation	1472	1482	1479	1478
v ₉	1590	NH_3^+ degenerate deformation	1590	1592	1592	1592
v ₁₀	2820	combination	2820	2823	2824	2829
v ₁₁	2895	combination	2895	2893	2893	---
v ₁₂	2965	CH_3 symmetric stretching	2965	2965	2965	2967
v ₁₃	3032	CH_3 degenerate stretching	3032	3034	3036	---
v ₁₄	3039	CH_3 degenerate stretching	3039	---	---	---
v ₁₅	3105	NH_3^+ symmetric stretching	3105	3105	3107	---
v ₁₆	3144	NH_3^+ degenerate stretching	3144	---	---	---

Fig. S3 Assignments of Raman bands of $\text{CH}_3\text{NH}_3\text{PbBr}_3$.¹

4. Temperature dependence of the peak positions of the Raman bands of MAPbBr₃.

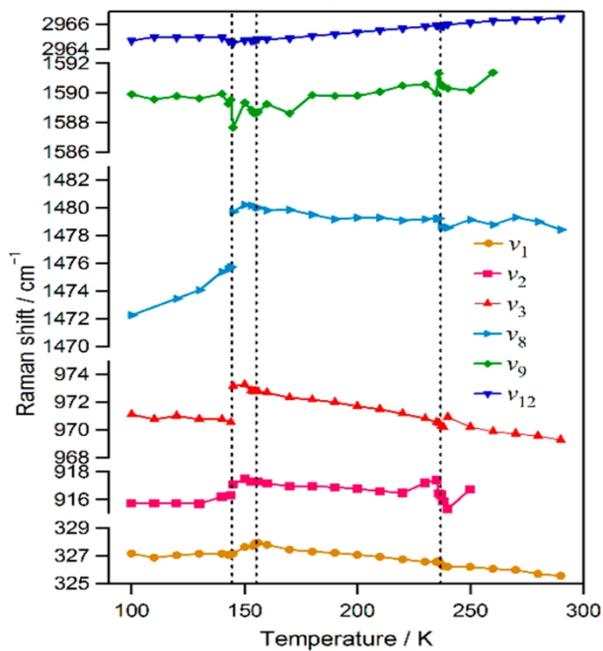


Fig. S4 Temperature dependence of the peak positions of the Raman bands of MAPbBr₃.¹

5. The electrode structure of MAPbBr₃ SC

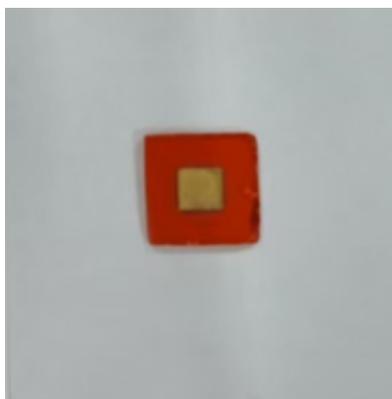


Fig. S5 The electrode structure of MAPbBr₃ SC

References

- 1 K. Nakada, Y. Matsumoto, Y. Shimoi, K. Yamada and Y. Furukawa, *Molecules*, 2019, **24**, 626.