Characterization of Organic Halide Perovskite by FTIR, Raman, and PL Spectroscopies

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Abstract Hybrid organic inorganic perovskite (HOIP) has become an important emerging material for solar cell research due to its simple and low-cost production and the capability to achieve high power conversion efficiency. Here we selected four commonly studied HOIP samples: FAPbI₃, FAPbBr₃, MAPbI₃, and MAPbBr₃ (FA=Formamidinium and MA=methylammonium) to investigate their optical properties. FTIR, Raman, and PL spectroscopy were performed and compared for the four samples. We find that the spectral features of FTIR can distinguish the organic part (FA or MA) of the HOIP samples, while the spectral features of Raman measurements can be used to analyze both the organic and inorganic part of HOIP. Furthermore, the FTIR and Raman spectra show several similar peaks from the organic part. Finally, the PL spectra are sensitive to the sample preparation method.

Hybrid organic inorganic perovskite



(a)

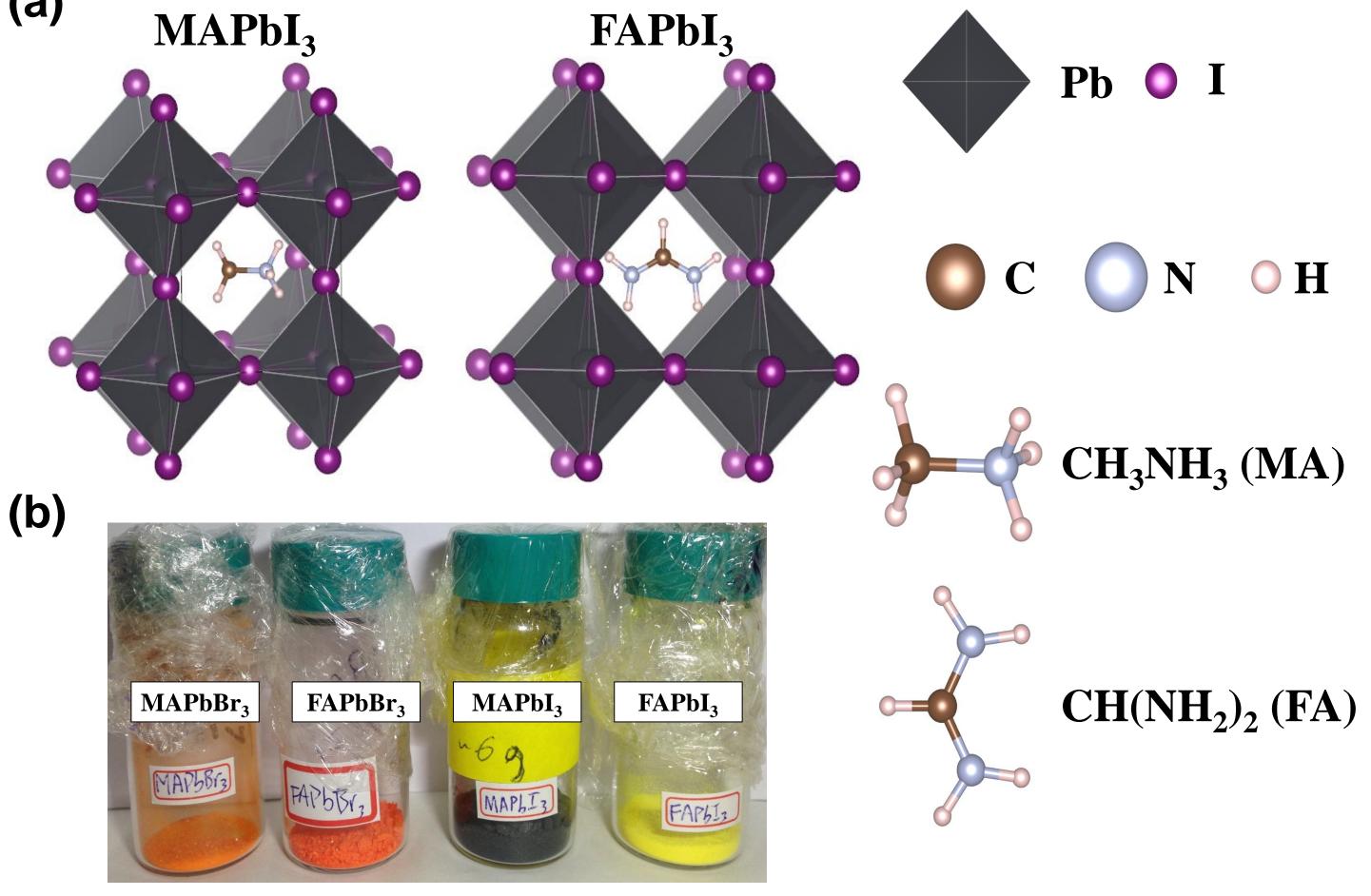


Figure 1 (a) Crystal structure of MAPbI₃ and FAPbI₃ perovskite. (b) Powder samples of MAPbBr₃, FAPbBr₃, MAPbI₃, and FAPbI₃.

FTIR and Raman measurements

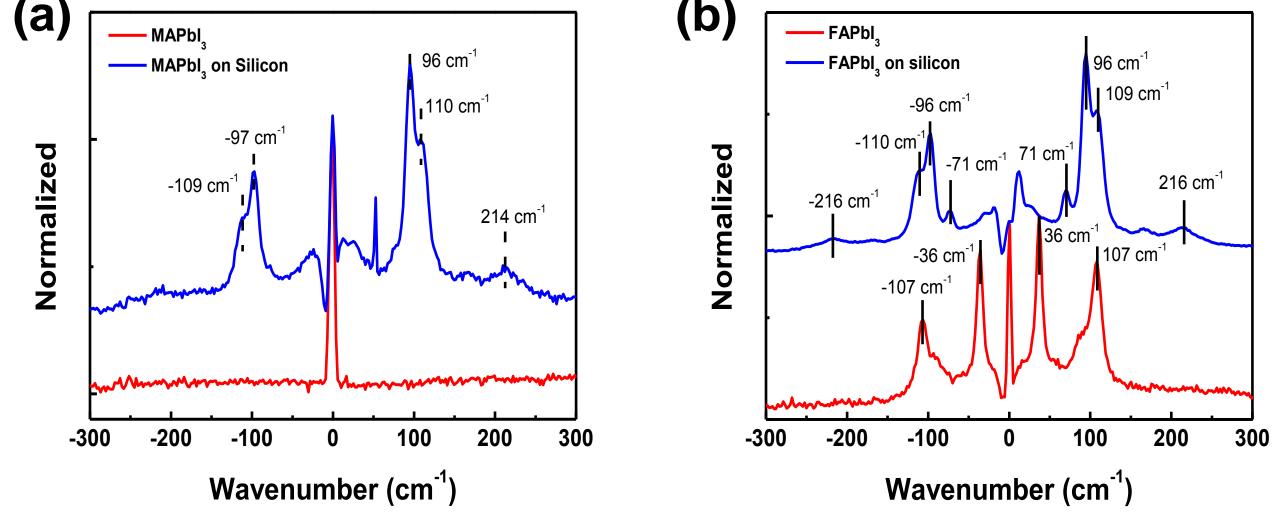
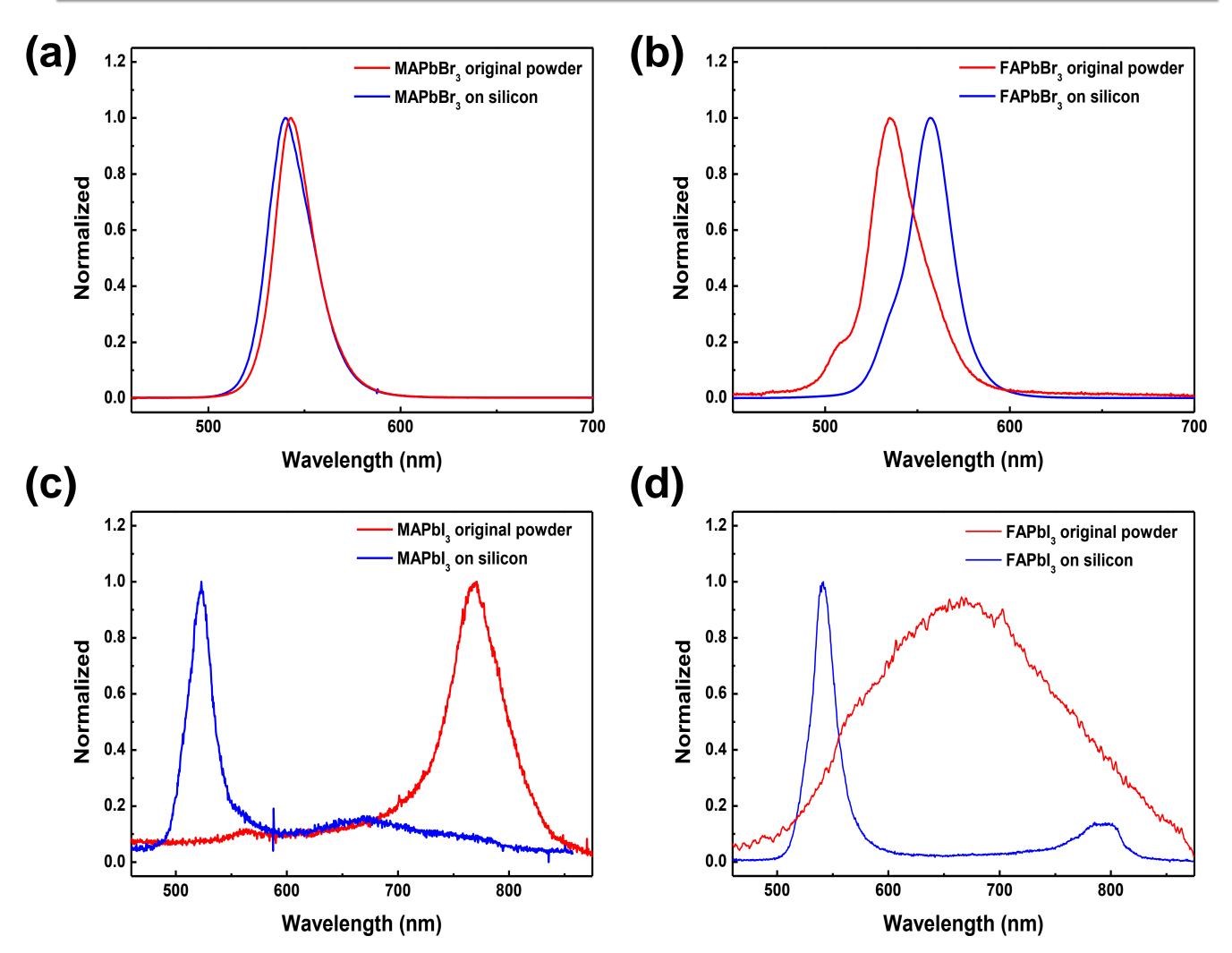


Figure 3 532 nm THz Raman measurement of (a) MAPbI₃ and (b) FAPbI₃. The low wavenumber Raman shifts are associated with the inorganic part of HOIP. The red lines are the spectra of powder or crystal samples, and the blue lines are the spectra of samples prepared by dispersing powder sample in 95% ethanol then dried on silicon. In (a) and (b), the peaks at about 71, 96, 110, and 214 cm⁻¹ are typical Raman features associated with PbI₂ [5]. Presence of these features indicates the degradation of the iodide samples.

Photoluminescence measurement



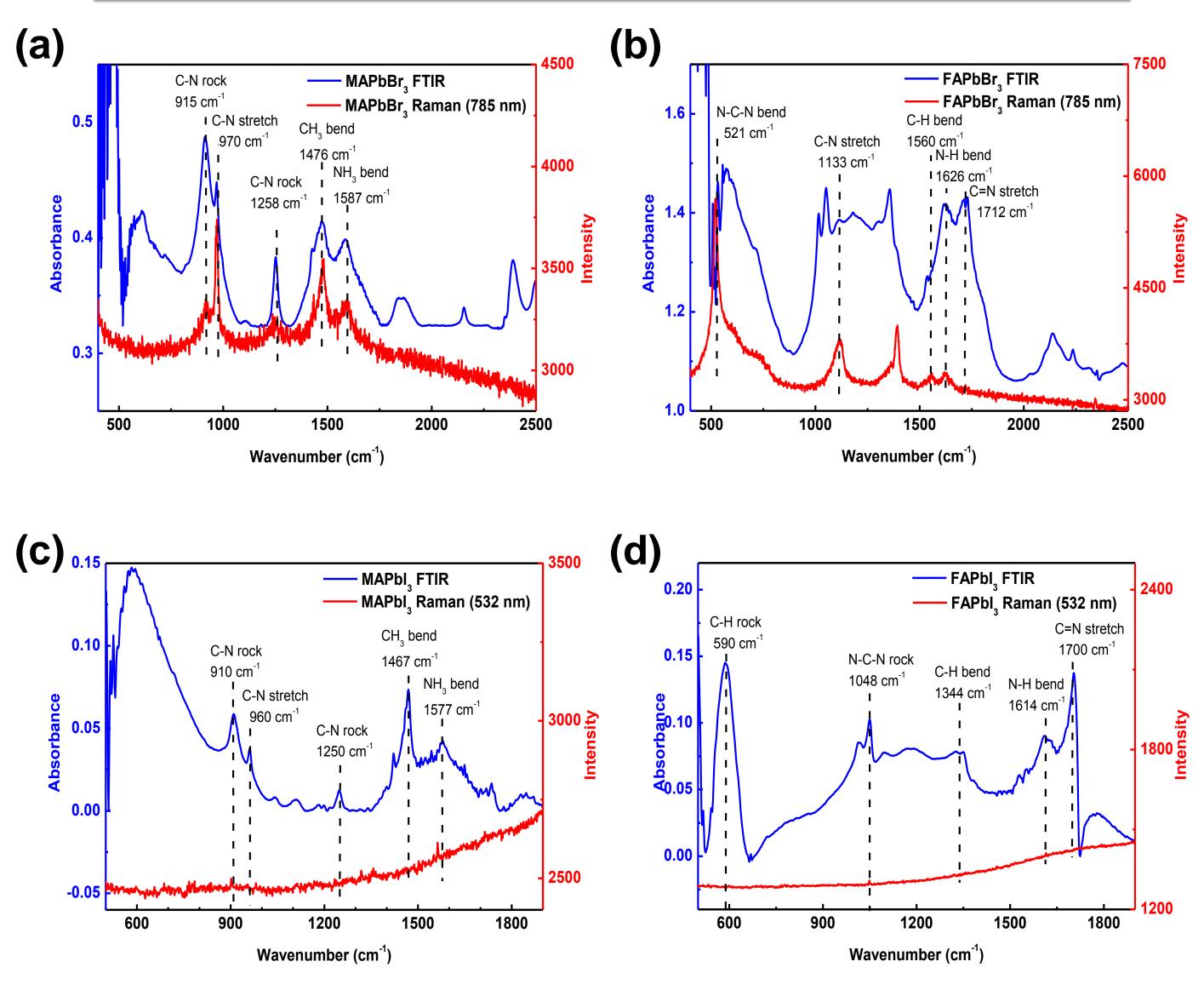


Figure 4 PL spectra of (a) MAPbBr₃, (b) FAPbBr₃, (c) MAPbI₃, and (d) FAPbI₃ excited by 450 nm laser. The red lines are the spectra of powder samples and blue lines are the spectra of samples prepared by dispersing powder samples in 95% ethanol and dried on silicon. In (a) and (b), the peak shifts can be observed in the spectra of the ethanol dispersed samples. In (c) and (d), the change of PL spectra indicates the degradation of the iodide sample, where the material structures change from MA(FA)PbI₃ to PbI₂.

Figure 2 Raman and FTIR spectra of (a) MAPbBr₃ (b) FAPbBr₃ (d) FAPbI₃ (c) MAPbI₃. Raman features from organic part of MAPbI₃ and FAPbI₃ were not observed in (c) and (d). In (a) and (c), 10 cm⁻¹ shifts of peak can be observed. The peak assignments are from reference [1-4]

Reference

[1] Ralf G. Niemann et al., J. Phys. Chem. C, 120 (5), pp 2509-2519, (2016) [2] Tobias Glaser et al., J. Phys. Chem. Lett., 6, pp 2913-2918, (2015) [3] Lingrui Wang et al., J. Phys. Chem. Lett., 7, pp 2556-2562, (2016) [4] E. Kucharska et al., *Vib. Spectrosc.*, 75, pp 45-50, (2014) [5] M. Y. Khilji et al., J. Raman Spec., 13, pp 127-133, (1982)

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Summary

	MAPbBr ₃	FAPbBr ₃	MAPbl ₃	FAPbl ₃
FTIR	Vibration modes from organic part can be observed			
532 nm THz Raman	Not observed due to strong PL at 500-600 nm		Only signal from Pbl ₂	Peaks from inorganic part observed
785 nm Raman	Some peaks from organic part similar to FTIR results		Not observed due to strong PL at 800 nm	
450 nm PL	Peak shift with different sample preparation		PL sensitive to the sample degradation	