

An in-situ infrared spectroscopy study on the influence of ALD SnO₂ on formamidinium-based metal halide perovskite

A.E.A. Bracesco¹, J.W.P. Jansen¹, W.M.M. Kessels^{1,2}, V. Zardetto², M. Creatore^{1,2}

¹Department of Applied Physics, Eindhoven University of Technology (TU/e), 5600 MB Eindhoven, The Netherlands

²Solliance, High Tech Campus 21, 5656 AE Eindhoven, The Netherlands

Supplementary information:

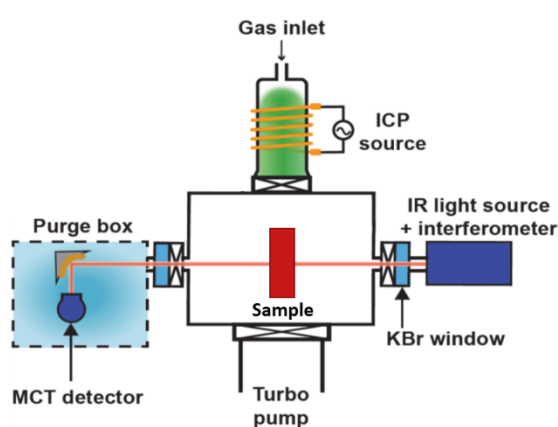


Figure 1: Schematic representation of the in-house built ALD reactor used for the experimental evaluation, with the in-situ IR setup and the positioning of the sample during the measurements. [Reproduced and modified with permission from M.J.M. Merckx, *Chem. Mater.* 2020, 32, 8, 3335–3345, 2020]

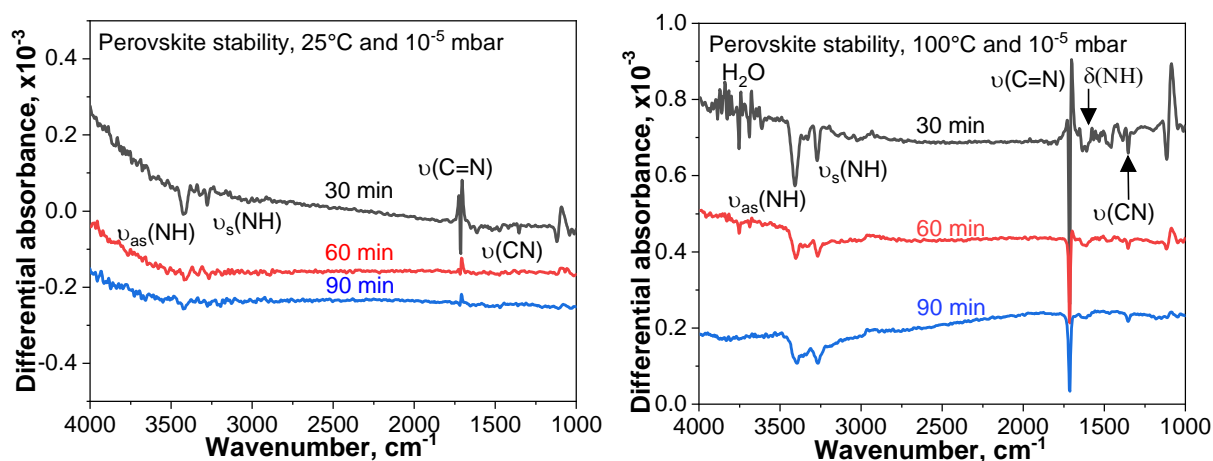


Figure 2: (Left): Evolution of the FTIR spectra during prolonged exposure of the perovskite to vacuum (10⁻⁵ mbar) at room temperature. (Right) Evolution of the FTIR spectra during prolonged exposure of the perovskite to heat (100°C) and vacuum (10⁻⁵ mbar). "Differential absorbance" indicates that each trace corresponds to the difference in absorbance between the spectrum measured under specific conditions and the spectrum of pristine perovskite at the start of the measurements. Negative peaks indicate the abstraction, or decomposition, of formamidinium cations from the perovskite surface. Positive peaks correspond to chemical modifications induced to the environment of the C=N bond in formamidinium, accompanied by a shift in frequency of the vibrational mode.

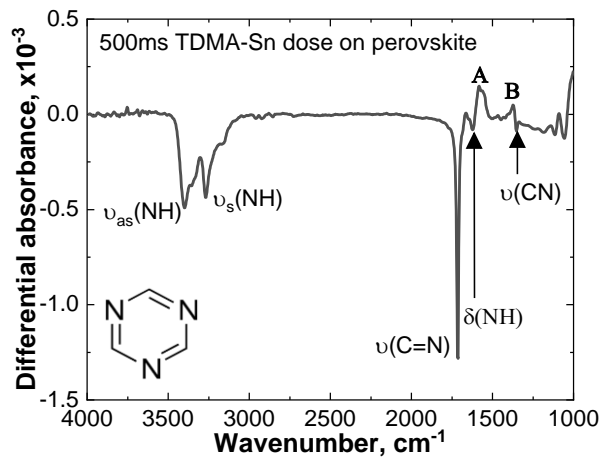


Figure 3: FTIR spectrum corresponding to the exposure of the $\text{CsFAPb}(\text{I},\text{Br})_3$ perovskite to one half-cycle of TDMA-Sn dose (500 ms) at a temperature of 100°C and at a pressure of 10^{-5} mbar. The vibrational modes associated to the formamidinium cations indicate their abstraction. “A” and “B” features correspond to the in-plane stretching of the sym-triazine molecule.