MS18-P05 | Combination of EXAFS and XRD for studies of the orthorhombic-tetragonal phase transformation in $MAPbI_{3-x}Cl_x$ perovskites

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Research interest has increasingly focused on hybrid perovskites $MABX_3$ like $[CH_3NH_3]^+$ (MA), B = Pb and X = I or Cl as a future photovoltaic material. In QENS studies it could be shown that chlorine substitution has a large influence on the rotational dynamics of the MA molecule in $MAPbI_{3-x}Cl_x$ perovskites. The QENS results show that chlorine substitution in the low temperature orthorhombic phase leads to a weakening of the hydrogen bridge bonds (these bonds connect the MA molecules with the $[PbX_6]^-$ octahedra host structure) since the characteristic relaxation times of C_3 rotation at 70 K in $MAPbCl_3$ (135 ps) and $MAPbI_{2.94}Cl_{0.06}$ (485 ps) are much shorter than in $MAPbI_3$ (1635 ps).[1] The structural counterpart to the changes in the MA molecule dynamics caused by the chlorine substitution is the influence of the chlorine substitution on the tilting and distortion of the $[PbX_6]^-$ octahedra in the orthorhombic-tetragonal phase transformation temperature range. By a combination of EXAFS Pb L3 edge investigations (local structure) and XRD (long-range order) the influence of the chlorine substitution on the distortions of the $[PbX_6]^-$ octahedra was investigated. The temperature dependent XAFS measurements as well as the temperature dependent XRD measurements were performed at KMC-2 at Bessy II.

[1] G. Schuck, F. Lehmann, J. Ollivier, H. Mutka, S. Schorr, J. Phys. Chem. C (2019), DOI: 10.1021/acs.jpcc.9b01238.