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EXAFS Studies of Mulfiferroic Pb(Ti,Fe)O₃ YING ZOU, SOMA-DITYA SEN, SHISHIR RAY, MARK WILLIAMSEN, University of Wisconsin-Milwaukee, USA, TOMOHIRO SHIBATA, SOMA CHATTOPADHYAY, Illinois Institute of Technology, USA, MALI BALASUBRAMANIAN, APS-Argonne National Laboratory, USA, PRASENJIT GUPTASARMA¹, University of Wisconsin-Milwaukee, USA — Recent suggestions [1] of multiferroic behavior in Pb(Ti,Fe)O₃ has revived an interest in this text-book ABO₃ type ferroelectric material. Here, we study the effect of Fe-substitution on the local structural and chemical environment of the parent PbTiO₃ phase. We have carried out extended x-ray absorption fine structure (EXAFS) measurements at the Fe-K, Ti-K and Pb-LIII edge at the Advanced Photon Source, on a series of single phase samples of $PbTi_{1-x}Fe_xO_3$ (0< x < 0.5) synthesized using a sol-gel technique. The near edge fine structure (XANES) reveals that Fe cations are trivalent. A fascinating new result is the observation of charge disproportionation of Pb into Pb2+ and Pb4+, likely a result of charge redistribution arising from Fe3+ substitution. Radial distribution function (RDF) study of EXAFS spectra from the Ti-K edge and the Fe-K edge confirms that Fe substitutes Ti up to x=0.5. 1. Palkar et al, Appl. Phys. Lett. 90(2007)172901.

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