Abstract Submitted
for the MAR10 Meeting of
The American Physical Society

Local distortions with the substitution of Se for Te in $FeSe_{0.5}Te_{0.5}$
DESPINA LOUCA, University of Virginia, K. HORIGANE, Tohoku University, A. LLOBET, Los Alamos National Kaboratory, R. ARITA, University of Tokyo — The isovalent substitution of Te for Se in the superconductor $FeSe_{1-x}Te_x$ increases T_c in comparison to α-FeSe but, on average, decreases the chalcogen-Fe bond angle. However, we find that the local symmetry is lower than the one presumed on average, *P4/nmm*, because the Se and Te ions do not share the same site, and have two distinct textitz-coordinates exhibiting two types of bond angles and bond lengths with Fe. Simultaneously, ab-initio calculations based on spin density function theory yielded an optimized structure with distinct z -coordinates for Se and Te, in agreement with the experiment.

Despina Louca
University of Virginia

Date submitted: 07 Dec 2009 Electronic form version 1.4