

Abstract Submitted
for the MAR07 Meeting of
The American Physical Society

***Ab Initio* XAS Debye-Waller Factors Beyond the Harmonic Approximation** FERNANDO VILA, University of Washington, H. H. ROSSNER, H. J. KRAPPE, Hahn-Meitner-Institut, J. J. REHR, University of Washington — We introduce an *ab initio* approach to calculate the temperature dependent vibrational effects in x-ray absorption spectra beyond the harmonic approximation. Instead of relying on empirical models, we apply electronic structure theory to determine the dynamical matrix of the system, from which the appropriate vibrational densities of state can be obtained using a Lanczos recursion algorithm [2]. By combining thermodynamic perturbation theory and the quasi-harmonic approximation we obtain x-ray absorption fine structure (XAFS) cumulants such as the mean square relative displacement (2nd cumulant), the thermal expansion (first cumulant), the asymmetry of the distribution (third cumulant) and the perpendicular motion contribution to the DW factor. Other quantities of interest such as mean square atomic displacements are also discussed. [2]H.J. Krappe and H.H. Rossner, Phys. Rev. **B70**, 104102 (2004).

Fernando Vila
University of Washington

Date submitted: 20 Nov 2006

Electronic form version 1.4