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***Ab initio* X-Ray Absorption Fine Structure Cumulants**[1] F. VILA, J.J. REHR, University of Washington, H.H. ROSSNER, H.J. KRAPPE, Hahn-Meitner-Institut — Theoretical calculations of vibrational effects in x-ray absorption spectra typically employ semi-phenomenological models, e.g. empirical force constants or correlated Debye or Einstein models. Instead we introduce an efficient and generally applicable *ab initio* approach based on electronic structure calculations of the dynamical matrix together with the Lanczos recursion algorithm [1] and relations between the cumulants. The approach yields 1) the thermal expansion coefficients (first cumulant of the vibrational distribution function); 2) correlated Debye-Waller factors (second cumulants) and 3) anharmonic contributions (third cumulants). Results are presented for crystalline (Cu, Au, Ge, GaAs) and molecular ($GeCl_4$, C_6H_6) systems. Our results for the Debye-Waller factors agree well with experiment.

[1]H.J. Krappe and H.H. Rossner, Phys. Rev. B**70**, 104102 (2004).

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