The Effects of Quantum Nuclei on Near-edge X-ray Spectroscopy in Crystalline Solids

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The simulation of spectroscopy for a material requires an accurate understanding of the atomic positions and structure. Even for crystalline solids where the atoms have well defined equilibrium positions, vibrations around those positions can have a profound effect on the near-edge x-ray absorption and emission. We show that not only thermally excited phonon modes, but also the zero-point vibrations, must be taken into account. As an example we compare measurements and calculations of the nitrogen K-edge absorption and resonant inelastic x-ray scattering for ammonium chloride, highlighting the effect of disorder of atoms in a crystal.