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Effects of asphericity in charge distribution on electron scattering amplitude.[1] JIN-CHENG ZHENG, LIJUN WU, YIMEI ZHU, Brookhaven National Laboratory, Upton, NY 11973 — The sensitivity of atomic scattering factors to valence-charge distributions has been compared quantitatively for x-ray and electron diffraction. It is found that electron diffraction provides information about valence charge densities via the low-order structure factors, which are relatively insensitive to thermal vibrations, but sensitive to the charge distribution that characterizes the chemical bonding properties in materials. The effects of asphericity in charge distribution on electron scattering amplitude have been examined using both analytical and numerical methods. We show that the aspheric effects are dominated in low-order scattering region, where the electron scattering factor of Bragg reflections can be measured very precisely by quantitative electron diffraction, and therefore enables us to quantitatively determine the spherical and aspherical orbital ordering. The applications of quantitative electron diffraction in strongly correlated materials are discussed.

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