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Electron structure factor: a unique quantity in probing material's properties.¹ JIN-CHENG ZHENG, LIJUN WU, YIMEI ZHU, Center For Functional Nanomaterials, Brookhaven National Laboratory, Upton, New York 11973 — Electron diffraction is very sensitive to valence charge distribution compared with x-ray at small scattering angles due to the near cancellation of the scattering from the positively charged nucleus and the negatively charged electrons. Thus, small changes in electron density can lead to considerable variations in the scattering amplitude. The well known divergence at small scattering vector for Coulomb scattering leads to strong measurable scattered intensities. However, the advantage of the accurate measurement using quantitative electron diffraction has not been well appreciated. We propose here that the accurate measured electron structure factor can be a unique quantity in probing properties of materials. We demonstrate this by examining the sensitivity of electron structure factor to valence charge distribution, chemical composition variations, and charge / orbital orderings in many functional materials. We also show that the accurately measured low-order electron structure factors can be used to test first principles theories, especially to optimize exchange-correlation functionals.

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