Poster

The charge density derived from electron diffraction on simulated data differs from that obtained from X-ray diffraction

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3D electron diffraction (3D ED) or microcrystal electron diffraction (MicroED), has become a complementary to X-ray diffraction technique for determining the routine crystal structure of compounds from sub-micron size crystals[1-3]. Moreover, electron diffraction can also provide high-resolution high-good quality data but charge density analysis of that data is still very challenging. On the other hand, the field of charge density analysis on X-ray diffraction data is well-established.

Here, we present the charge density analysis on simulated electron and X-ray diffraction data. We computed both simulated electron and X-ray diffraction structure factors for a number of organic crystals using periodic DFT approach. Next, we developed proper strategy for the multipole model refinement for these organic crystals. Finally, we examined the resulting charge density models. It appeared that the charge density models derived from electron diffraction significantly differ from that obtained from X-ray diffraction. In particular, the models have different atomic charges, expansion-contraction parameters, populations of higher mutlipoles, deformation densities, electrostatic potentials, and topological properties. Ultimately, we want to determine which charge density models, the ones from electron diffraction or the ones from X-ray diffraction represents the original charge density obtained directly from periodic DFT.

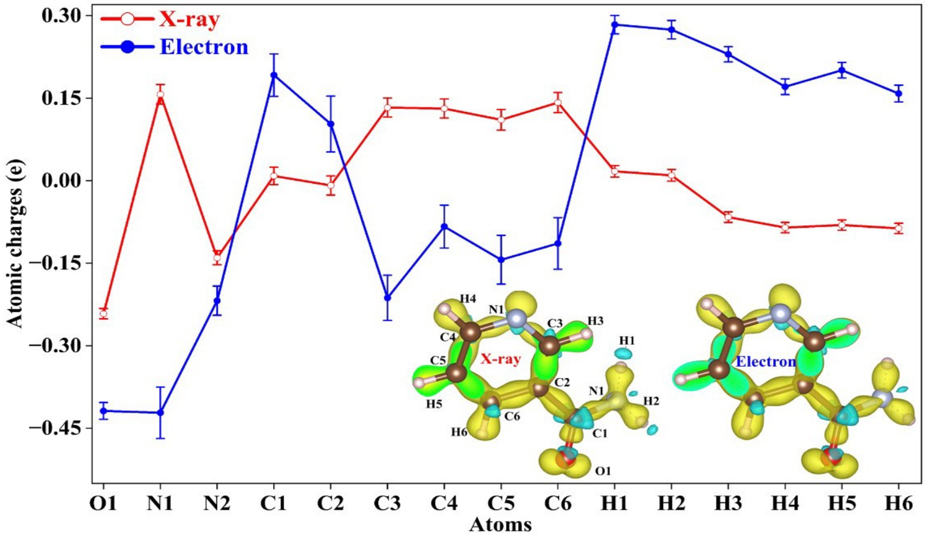

Figure 1. Atomic charges derived from valence electron populations and deformation electron density maps from X-ray (red) and electron (blue) diffraction data computed for nicotinamide crystal.

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