Multipole modelling in electron diffraction studies

Ashwin Suresh

Institute of Physics of the CAS, Prague, Czech Republic

The use of single-crystal diffraction experiments for crystal structure determination has been extensively explored over the years. These experiments are often limited to the determination of the three-dimensional structure of the studied compound by deducing the positions of atomic nuclei in the unit cell. Most methods used to determine the crystal structures rely on a simple model called the 'Independent Atom Model' (IAM), which assumes the crystal to be an assembly of non-interacting atoms and the corresponding electrostatic potentials and electron densities to be spherical and centred on the coordinates of the corresponding nuclei.[1] Although IAM is a reasonable starting point and it is acceptable to build a reasonably correct structural model, it is chemically inconsistent lacking the typical features of chemical bonding.[2,3]

Alternative models to IAM have been studied in the past to extract fine electron density features from exceptionally good-quality X-ray data.[3] In the seminar, I will try to summarize the different models for charge density analysis and also explore the possibilities to use these models with data collected from electron diffraction experiments.

*corresponding author: e-mail: ashwinsuresh650@gmail.com

References

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