

Beyond Visual Inspection: Evaluating Imperfect Symmetry in Crystals

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Symmetry and chirality are fundamental properties of crystals, often discussed in categorical terms while overlooking the rich world of approximately symmetric structures. The challenge lies not only in developing computational tools to quantify these properties but also in ensuring their meaningful application. The Continuous Symmetry Measure (CSM) and Continuous Chirality Measure (CCM) provide a robust numerical framework for assessing structural deviations, offering a powerful lens through which to analyse molecular geometry [1–3]. This approach encourages us to examine whether structural deformations are purely inevitable consequences of environmental influences or if they serve a functional, intentional role in molecular systems. Nevertheless, their interpretation requires careful consideration as numerical distortion levels do not always align with immediate visual or conceptual expectations. This lecture will explore the advantages and challenges of applying CSM and CCM to analyzing crystals, with specific examples that highlight the additional insights these methods offer to expand our perspective on crystal structures.

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- [2] G. Alon, Y. Ben-Haim, and I. Tuvi-Arad, Continuous symmetry and chirality measures: approximate algorithms for large molecular structures, *J. Cheminform.* 15, 106 (2023).
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