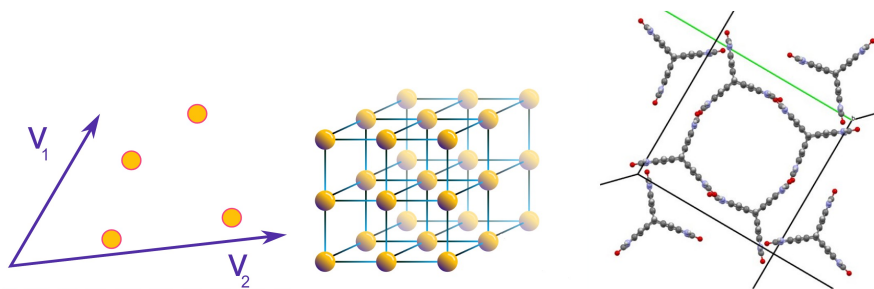# An Introduction to Mathematical Crystallography

26th November 2025

Abstract: Crystallography is the study of solid crystalline materials (periodic crystals). This talk will introduce a new geometric approach to a mathematical definition of a crystal structure.

Chemists dream of designing a new material that would change the world, such as a room-temperature superconductor, or a photocatalyst for hydrogen fuel. Recently, AI tried to predict new materials by generating millions and millions of simulated crystals, but failed to recognise thousands of exact duplicates and many more near-duplicates among their predictions.

We will discuss how the emerging field of Geometric Data Science develops continuous metrics to rigorously study real objects in crystallography and beyond.

Speaker: **Tatiana Kurlina**

Location: Room 105, 24 Gordon Square
Time: **1.30-2.30pm**