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One million structures to power chemical science

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For over 50 years, the Cambridge Crystallographic Data Centre (CCDC) has been curating the world's small molecule crystal structures into the Cambridge Structural Database (CSD). This collection has grown steadily through the years and is now poised to reach 1 million structures. Far more than just a collection of crystal structures, the data in the CSD provide the fuel that drives scientific discovery across diverse areas of research. This presentation will focus on a number of research projects that incorporate the software tools that harness the power of the CSD. We will look at methods that explore the crystallographic solid form of small molecules by elucidating intermolecular interaction networks, from hydrogen to halogen bonding, assessing the risk of polymorphism and understanding molecular geometries.

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