GI-MS48-04 | Crystal Structure Exploration – I didn't Know Mercury Could Do That!

Stevens, Joanna (The Cambridge Crystallographic Data Centre, Cambridge, GBR); Maloney, Andrew (The Cambridge Crystallographic Data Centre, Cambirdge, GBR)

It's been an 18-year journey from leaving Pluto for Mercury, the original to current version (4.0) of the CCDC's visualisation software – and it's come a long way, having boldly gone beyond its original mission as a simple package for the display of crystal structures.

Mercury has developed into a powerful platform, encompassing a wide range of structural analysis and visualisation capabilities, delivering analysis, design and prediction functionality. This includes the ability to easily examine interactions and symmetry elements, structure editing and overlaying of structures, through to tools for assessing and ultimately gaining insights in different aspects such as hydrogen bonding, conformation and packing. This is not to mention the interactive data analysis functionality and interfacing with results from searching the Cambridge Structural Database, the collective repository for small-molecule organic and metal-organic crystal structures.

This presentation will highlight some of the less well known, underutilised or simply overlooked features within Mercury, in order to more effectively explore your crystal structures and the universe of crystallography.

[1] Mercury CSD 2.0 – new features for the visualization and investigation of crystal structures, C. F. Macrae, I. J. Bruno, J. A. Chisholm, P. R. Edgington, P. McCabe, E. Pidcock, L. Rodriguez-Monge, R.Taylor, J.van de Streek and P. A. Wood.,J. Appl. Cryst., 2008, 41, 466–470, DOI: 10.1107/S0021889807067908
[2] The Cambridge Structural Database, C. R. Groom, I. J. Bruno, M. P. Lightfoot and S. C. Ward, Acta Cryst., 2016, B72, 171-179, DOI: 10.1107/S2052520616003954