

Metal-organics: A rich seam of data for knowledge mining

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In the last year, the Cambridge Structural Database (CSD) has grown to encompass over 875,000 entries and it could potentially reach a million entries before the next ACA meeting in 2018! As the number of entries has increased in recent decades, the fraction of metal-organic entries has steadily increased, accounting for more than half of the CSD since 1991 and reaching 57% of all entries at the start of 2017. Despite this abundance of structural data on metal-organic systems, there is still relatively little research in detailed structural analysis, design and prediction of metal-organic compounds compared to the purely organic field. We think this area has a lot of potential for effective use of knowledge-mining concepts and applications.

Here we will present some of the improvements currently being made to the CSD software to aid searching, visualisation and analysis of metal-organic structures as well as ideas for what to do next. This is also a partially crowd-sourced poster as we will be encouraging you, the ACA community, to give your thoughts on what else we should improve and what the highest priority should be!