

FUNCTIONALIZATION OF MOLYBDENUM BLUE POLYOXOMETALATES WITH AMINO ACIDS AND PEPTIDES

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Polyoxometalates (POMs) are metal-oxygen clusters with diverse properties and structures. Molybdenum Blue (MB) is a subgroup of polyoxometalates of the largest known molecular structures with up to 368 Mo atoms contained in a single cluster. Since their crystal structures were first unveiled in the 1990's [1], major interests focused on the assembly and characterization of MB-organic hybrids with organic guests via supramolecular interactions. We recently reported a series of work on covalent modification of MBs with amino acids and peptides [2-5]. In this contribution, we demonstrate a workflow that can be tracked manually or by a robot and use it for the discovery of new MBs that are composed of various types of amino acid ligands. In a systematic search of reaction conditions in a fixed range, we identified a number of the $\{\text{Mo}_{154}\}$ MB clusters with different crystal structures forming 1-D arrays or 2-D sheets (Figure 1). Detailed experimental designs with robotic control and data illustrations are present.

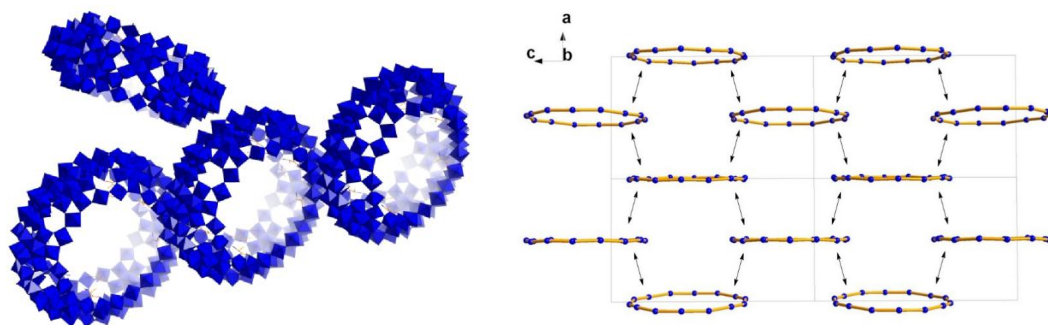


Figure 1. Left: 1-D array of $\{\text{Mo}_{154}\}$ MB clusters observed in a new phase of MB-amino acid hybrid; Right: Representative packing diagram indicates 2-D layer structures of $\{\text{Mo}_{154}\}$ clusters on crystallographic ac plane in another new phase. The dual arrows indicate the places of Mo-O-Mo bridges between $\{\text{Mo}_{154}\}$ wheels.

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