Constructing Novel Polymorphs from Nanoclusters taken from WASP@N

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The WASP@N project (Web Assisted Structure Prediction at the Nanoscale) is essentially the creation of a searchable website database of atomic structures of nanoclusters. The database, or HIVE, has been developed for the nanocluster community including those who actively predict local minima (LM) structures and also those who require atomic structure information in order to begin their simulations/ investigations. The WASP@N interface enables the easy visualization and comparison between nanoclusters. Led by myself, this project benefits from the talents of T Lazauskas, A Sokol, and M Zwijnenburg (UCL, UK), M Illingworth, and A Carter (EPCC, UK), R Johnston (Birmingham, UK), S Bromley (Barcelona, Spain), J Gale (Curtin, Australia), V Blum (Duke, US), and J Bel Bruno (Dartmouth, US) and is supported by EPSRC.

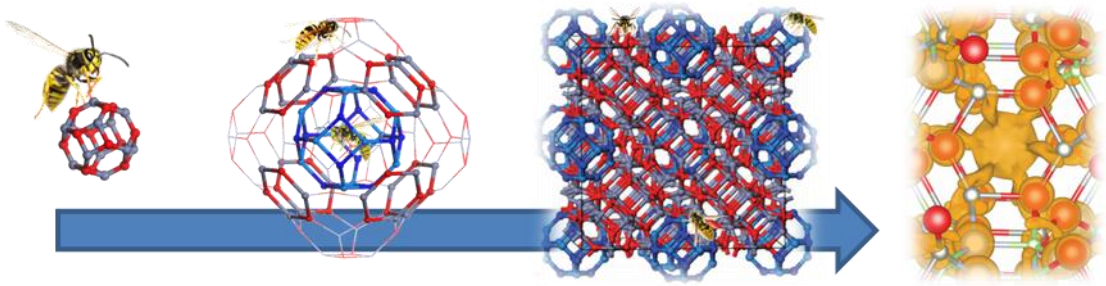

Figure 1. Two T_h nanoclusters are combined and then used as a secondary building unit to form a novel polymorph. The compound for each nanocluster is then selected to optimize the desired electronic property of the bulk phase.

Novel and some familiar microporous framework polymorphs have been constructed from high symmetry 1:1 LM nanoclusters taken from the HIVE. For the selected compounds, high symmetry LM are typically the global minima for their respective size; we have investigated secondary building units with point symmetry T_h and T_d, which are formed of three coordinated atoms that make a layer of hexagons that is curved in 3D by the presence of six tetragons. In these SBUs, the distance between the tetragons is maximized (they are only edge sharing in the smallest T_d nanocluster, which is a cube of only tetragons). Clearly, stacking the cuboids will generate the well known NaCl rock salt polymorph, whereas using larger SBU can generate polymorphs containing larger pores. Initially we considered the stability of polymorphs as a function of density and then chose compounds in order to tune a desired property.

Bibliography

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