

Nets, Tilings, Topological Crystal Chemistry and designed Synthesis of Porous Materials

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Topics

Crystal structures and their description as nets

Some important inorganic structure types, metal-organic frameworks, zeolites,

Introduction to graph theory

Cycles, sums, rings, strong rungs; trees, cyclomatic number; planar graphs; polyhedra as graphs

Periodic graphs and nets

Crystal structures as nets; embeddability and sphere packings; quotient graphs; minimal nets; regular and semiregular nets; point and vertex symbols

Periodic tilings and nets

Natural tilings of nets; signatures; duals; self-dual tilings and their nets; transitivity

The RCSR database

Symbols for nets; searching the RCSR database

Using Systre

Barycentric coordinates; nets with collisions; graph input; crystal input; interpreting output

Using 3dt

Delaney symbols; TILING input; visualization of net and tiling; manipulating tiles; exporting graphics

Using TOPOS

Topological analysis, generating 3dt and Systre input

Deconstructing crystal structures:

MOFs, COFs, ZIFs and coordination polymers; zeolites; structure building units and points of extension

Periodic surfaces

Nets as periodic surfaces; genus; curvature; minimal surfaces; surfaces in chemistry (mesoporous materials etc)

Porous materials

Zeolites; zeolite-like oxide materials; MOFs, COFs and ZIFs

Note: The demonstrations will use the free programs Systre, 3dt and TOPOS. The first two work on any modern platform but TOPOS is restricted to Windows. Participants should have a portable computer (laptop) for full participation in the demonstrations

Course materials.

Attendees will get copies of all lectures and demonstration materials