



**Figure 1.** (a) Schematic representation of an imogolite nanotube; (b) X-ray scattering pattern of  $(\text{OH})_3\text{Al}_2\text{O}_3\text{GeOH}$  nanotubes, together with its simulation for the refined structure, showing the good agreement between experiment and simulation.

**Keywords:** Crystallography, imogolite

## MS15. Structure property relationships

Chairs: Kari Rissanen, Martin Bremholm

### MS15-O1 Design and synthesis of molecular materials: mixed crystals for finer engineering

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The properties of a material depend on both the nature of its constituents (*chemistry*) and the way they are arranged in the space (*structure*). Crystal engineering is the discipline that investigates and exploits the relationship between structure and physical properties to produce tailor-made crystalline molecular materials. A limitation to such activity is represented by the finite (*discrete*) nature of the molecular components (*building blocks*) that prevent the material's fine tuning. By combining the functions and sterics of multiple, equivalent building blocks crystalline solid solutions (*mixed crystals*), whose composition can be varied in continuum, provide an extra degree of control over the material's properties. Hence, for this class of compounds the crystal engineering problem would coincide with the synthesis of the appropriate mixed crystal. Unfortunately, traditional crystallisation techniques are likely to result in molecule separation precluding the formation of mixed crystal. Therefore solvent-free alternatives must be developed and pursued. Solid-solid and solid-gas reactions represent a viable alternative to wet chemistry in the production of homogeneous solid solutions of organic, metalorganic and organometallic species. This strategy has proved successful in engineering reactivity, polymorphism, photoemission spectra and unit cell metrics of a number of materials including coordination polymers, molecular sieves, dyes and pharmaceuticals.

**Keywords:** `crystal_engineering`, `solid_solutions`, `mixed_crystals`, `solid_state_reactions`