# The long-time elusive structure of magadiite, solved by 3D electron diffraction and model building

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Magadiite, $Na_2Si_{14}O_{28}(OH)_2 \cdot nH_2O$, is known as a mineral discovered at the lake Magadi in Kenya by Hans Eugster in 1967 [1]. Since then, magadiite-type materials have also frequently been synthesized in the lab and have come into focus for various applications [2-4], like $CO_2$ adsorbents, drug carriers or catalysts and maintain a rising interest.

Despite many attempts, the unique magadiite structure remained unsolved. Finally, a material-specific strategy based on 3D electron diffraction successfully deciphered the atomic structure [5]. In order to enable the *ab initio* structure solution of the electron beam sensitive material, a sodium-free dehydrated form of magadiite was synthetically isolated and, from that, it was subsequently possible to derive a structure model for the sodium form of magadiite, later successfully refined against *powder X-ray diffraction* data. Furthermore, a geometry optimization, simulations of spectroscopic data and calculation of charge transfer between the water molecules and the silicate layer with *DFT* methods confirmed the obtained crystal structure of sodium magadiite.

The structure of the silicate layer is quite complex, as it contains 4-, 5-, 6-, 7-, and 8-rings of three- and four-interconnected $[SiO_{4/2}]$ tetrahedra. Seven symmetrically independent Si atoms and 15 independent oxygen sites are present forming a dense layer of considerable thickness (11.5 Å). The symmetry can be described by the layer group *c*211. Each layer is chiral, but the chirality of the stacked silicate layers in the average structure (*F*2*dd*) is alternated, due to the glide plane perpendicular to the stacking axis. Bands of interconnected $[Na(H_2O)_{6/1.5}]^+$ octahedra are intercalated between neighbouring silicate layers to compensate the charge of the layers.

The detailed knowledge now achieved on the previously unknown silicate layer and the development of an adapted synthesis combined with an ammonia-based titration will have a huge impact on the research of hybrid organic−inorganic nanocomposites based on magadiite, related layered silicates and zeolite-like structures in order to design new and more efficient materials.

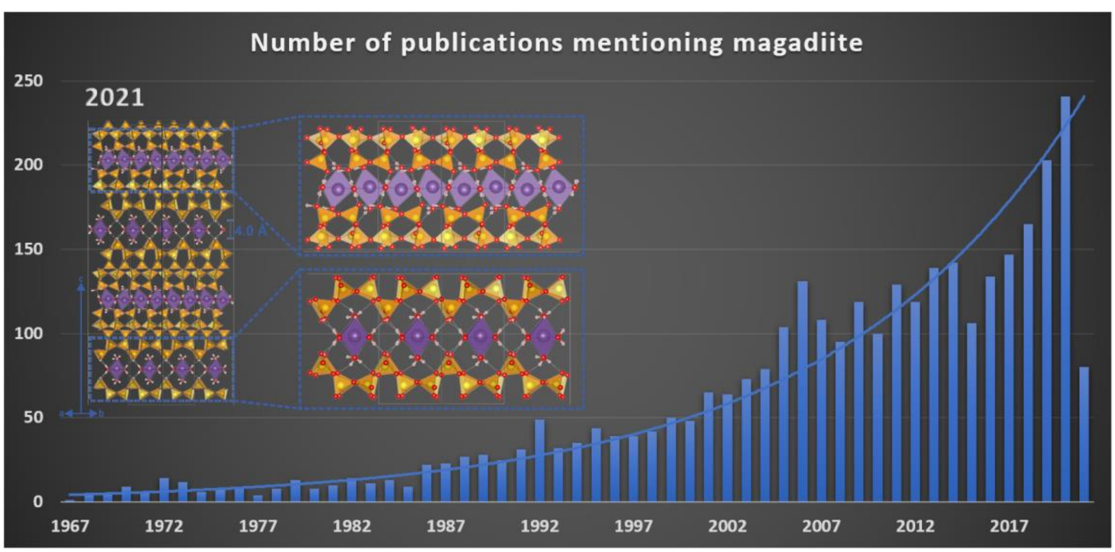


**Figure 1**. Number of publications mentioning magadiite. Inset illustrates the structure of sodium magadiite with view along [110].

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