

# Application of the Voronoi tessellation for high-throughput analysis of crystalline porous materials

Frontiers in Computation: New Methods for Complex Mechanics, Advanced Materials, Interfaces, and Stochastics

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## *Abstract*

Crystalline porous materials, such as zeolites, contain complex networks of void channels that are exploited in many industrial applications. Since the 1950s, they have been employed in common applications such as chemical catalysts and water softeners, and more recently there has been interest their use for new technologies such as carbon capture and storage. A key requirement for the success of any nanoporous material is that the chemical composition and pore topology must be optimal for a given application. However, this is a difficult task, since the number of possible pore topologies is extremely large: thousands of materials have been already been synthesized, and databases of millions of hypothetical structures are available.

We have developed tools for rapid screening of these large databases to automatically select materials whose pore topology may make them most appropriate for a given application. Many of the methods are based on computing the Voronoi network, which provides a map of void channels in a given structure. This is carried out using the free software library VORO++, which has been modified to properly account for three-dimensional non-orthogonal periodic boundary conditions.

The Voronoi network can be analyzed using Dijkstra-like graph algorithms to determine whether a molecule of a certain size can pass through a material. This calculation can then be coupled to a Monte Carlo sampling method to determine the amount of volume and surface area that is accessible to a molecule as it passes through the material. By simplifying the Voronoi networks, different materials be classified according to their pore topology. These algorithms have been implemented in the new software package ZEO++, which provides a suite of tools for the analysis and comparison of materials to match given requirements. Once the databases have been screened to identify the candidates that are most suitable for a given application, these materials can be analyzed further by using more detailed numerical techniques.