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The determination of new stable zeolite frameworks using a parallel hybrid genetic algorithm

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1 Introduction

Zeolites were originally discovered by the swedish mineralogist Axel Fredrik Cronstedt in 1756 [1]. However, it is only from the 1930s with Barrer pioneering work on the synthesis and adsorption properties of zeolites that the science of zeolites has really taken off [2]-[3]. Over the years 1950s the first processes for the synthesis of zeolites A, X and Y are developed before their commercialization by Union Carbide in 1954 [2]. The zeolites are crystalline microporous materials with outstanding characteristics of catalysis and adsorption. Zeolites are composed mainly of silicon (Si) and aluminum (Al) atoms which represent two of the most abundant elements on earth. The Zeolite Structures Problem (ZSP), so called by Falcioni and Deem [4], can be classified in the area of the computational chemistry [5]. The aim of this problem is to find optimal zeolite structures which depend on initial atoms positions.

Metaheuristics [6] are powerful heuristic algorithms capable of solving, among other problems, combinatorial and continuous optimization problems. The common characteristic of metaheuristics is to use a random mechanism to explore the space of solutions. Beyond the topology based methods, two major metaheuristics have been successfully exploited in the zeolite structures prediction: the former one is simulated annealing (SA) [7], used in particular for the crystal structure resolution from experimentally available data. The second, more recent, is the genetic algorithm (GA) [8].

2 Methods

Our proposition to solve the ZSP is a genetic algorithm hybridized with a heuristic based on the memorization and the prediction of the atoms positions. We have named this algorithm MEGA-HZ (from *MEmory Genetic Algorithm Hybridized for Zeolites*). The MEGA-HZ generates a random population. The oxygen atoms are added at the end of the algorithm to the center of two atoms T that can be connected. The aim of this algorithm is to find atoms positions to generate potential zeolite structures. The evolutionary algorithms are naturally adapted to propose original structures [9]. In this work, a distributed and massively parallel genetic hybrid algorithm is developed.

To create a viable zeolites by the MEGA-HZ, the algorithm needs to put the atoms at the right positions inside the AU. Each atom position of the Assymetric Unit (AU) is defined by 3 atomic coordinates (x,y,z). This step creates the AU. The symmetric operations defined in the space group are applied to the AU to generate the UC (Unit Cell). This UC is the smallest volume unit that contains all of the structural and symmetry information. Then, in order to form the bulk atoms arrangement of the crystals, the unit cells are stacked in the three-dimensional space. The objective is to generate viable zeolites frameworks taking into account the constraints determined by the user input.

3 Results

The MEGA-HZ algorithm found an unknown stable zeolite structure not recognized by the Structural Commission of the International Zeolite Association and the Atlas of Prospective Zeolite Structures [10, 11].

The unknown topology *HZM#4* has a three-dimensional pore system with 8 and 10 T atoms. One type of Composite Building Units (CBU) is observable ($[4^5 5^2]$ or *d5r*), these CBUs are connected with 4 tetrahedres to form pairs (Figure 1a). The arrangement of these pairs, separated from each other in space, gives rise to large cages ($[4^{12}5^4 6^2 8^4 10^2]$, Figure 1b), each large cage is linked to 8 pairs of CBUs *d5r* by pooling their cycles to 4 and 5 tetrahedron as shown in Figure 1c. Similarly, each pair of CBUs *d5r* is linked to 8 large cages ($[4^{12}5^4 6^2 8^4 10^2]$).

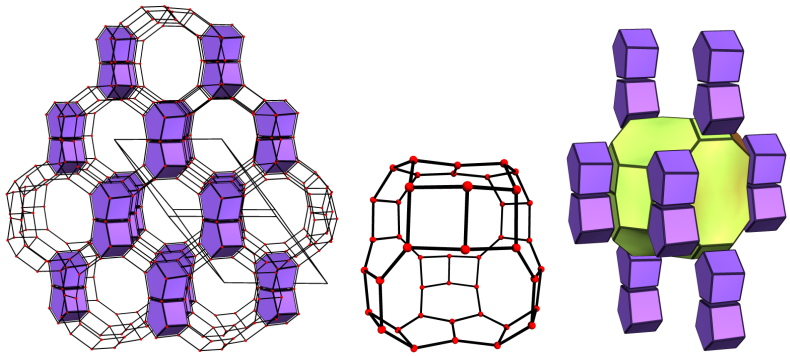

Fig. 1. 'Tiling' of the structure *HZM#4* showing (a) the spatial arrangement of CBUs pairs *d5r*, (b) a large cage $[4^{12}5^4 6^2 8^4 10^2]$ and (c) surrounded by 8 pairs of CBUs *d5r*. Oxygen atoms have been omitted for clarity.

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