



Using a novel parallel genetic hybrid algorithm to generate and determine new zeolite frameworks



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ABSTRACT

Zeolite structure determination and zeolite framework generation are not new problems but due to the increasing computer power, these problems came back and they are still a challenge despite the recent progress in terms of structural resolution from X-rays and electron diffraction. The infinite number of potential solutions and the computational cost of this problem make the use of metaheuristics significant for this problem. In this paper, we propose a new approach based on parallel genetic hybrid algorithm for zeolites using a modified modelization of the objective function to find hypothetical zeolite structures, close to the thermodynamic feasibility criterion. A population made of random atoms is initialized. At each generation, a crossover operator and a mutation heuristic are applied. Each individual of the population generates a potential zeolitic structure by applying the symmetry operators of a given crystallographic space group. This structure is evaluated with our objective function. From the unit cell parameters and the number of T atoms in the asymmetric unit, 6 possible zeolitic interesting structures have been found.

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1. Introduction

From the discovery of the first natural zeolite by the Swedish mineralogist Axel Fredrik Cronstedt (Cronstedt, 1756) to the most recent industrial applications, zeolites account for 250 years of history. Zeolites are crystalline microporous materials showing exceptional catalytic and sorption characteristics together and environmentally friendly. Their structures form micropores of molecular dimensions that contain exchangeable extra-framework cation. In the two centuries following this discovery, science of zeolites was limited only to natural zeolites discovered in large sedimentary basins. Note that it is almost impossible to have natural zeolites lots, homogeneous in composition and properties, considerably limiting their industrial use and reserving them for special

purposes directly related to people and their environment (insulating building materials, fish farming, livestock, etc.). It is only from the 1930s and Barrer pioneering work on the synthesis and adsorption properties of zeolites that the science of zeolites has really taken off (Barrer, 1982; Guisnet and Gilson, 2002). 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 (Barrer, 1982). At that time, these molecular sieves were used for drying, as catalysts in isomerization and cracking processes and also for separation of linear and branched alkanes. One of the challenges of research in the field of zeolites is the discovery of new usable microporous materials of zeolite-type. They are used for applications in catalysis, separation and adsorption.

It is particularly interesting for the oil industry to have new wide-pore zeolite catalysts to promote diffusion phenomena and/or to make new reactions with molecules larger in size. Zeolites are composed mainly of silicon (Si) and aluminum (Al) atoms which represent two of the most abundant elements on earth. Experimentally speaking, the synthesis of a new zeolite framework designed computationally is still the biggest challenge. For a large majority

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of cases, to synthesize a new zeolite, an organic structure directing agent (OSDA) is necessary. In terms of OSDA design, examples of the use of molecular modeling are rare, zeolite ZSM-18 being the most famous case (Schmitt and Kennedy, 1994). A more sophisticated method by Lewis et al. predicted an efficient OSDA that conducted to a molecular sieve having the chabazite topology in the aluminophosphate system (Lewis et al., 1997; Speybroeck et al., 2015). A similar methodology was developed by Pophale et al. (2013) and Schmidt et al. (2014). Both concepts are interesting but need further proofs in order to be considered as truly effective. Accordingly, the discovery of a novel zeolite is more or less serendipitous (Li et al., 2015) and it mostly remains a trial and error process. Nevertheless, a large effort has been devoted in the past decades to predict new zeolitic crystal structures. Started by the pioneering work of Wells (1954), the topology based approaches have been further applied by Smith (1977, 1978, 1979, 1988, 1989) and O’Keeffe (1991, 1995) who systematically enumerated the already existing and/or hypothetical zeolite structures. Analogical method of systematic enumeration, using tiling theory was successfully implemented by Foster et al. in order to identify thermodynamically feasible purely siliceous zeolites (Foster et al., 2004). The crystal structure modeling methods based on the topology principles are reviewed in detail by Woodley and Catlow (2008). Beyond the topology based methods, two major computational strategies have been successfully exploited in the zeolite structures prediction: the former one is simulated annealing (SA) (Pannetier et al., 1990) used in particular to the crystal structure resolution from experimentally available data. The second, more recent one is the genetic algorithm (GA) (Coley, 1998).

Genetic algorithms are useful to explore the search space and to find unexpected solution and have been successfully used to solve a problem from the computational chemistry, the so-called Lennard Jones (LJ) cluster problem (Bäck, 1996; Eshelman and Schaffer, 1993). For a given cluster of N atoms, the LJ cluster problem consists in finding the relative positions of atoms in the three dimensional Euclidean space at a minimum of the potential energy (Fan, 2002). Different works used also a genetic algorithm to solve the LJ cluster problem such as those published by Daven et al. (1996) and Barrón et al. (1999). This metaheuristic optimization method demonstrates a good ability to solve other chemical issues (Archibald et al., 2005). The ‘Zeolites Structure Problem’ (ZSP), so called by Falcioni and Deem (1999), is well within that concept. Beyond that, several complex inorganic solid structures have been successfully predicted through the GA combined to the force field based lattice energy minimization (Woodley et al., 1999). More recently, using GA, new feasible microporous framework structures have been generated based on exclusion zones approach (Woodley et al., 2004a,b). Baumes et al. have developed a methodology based on GA, after integration in the EASEA library (Collet et al., 2000) using a graphic processing unit (GPU) implementation (Baumes et al., 2011, 2013). Note that the last method was efficient to recover, for the most part, the complex interrupted framework of the meso-microporous silicogermanate ITQ-43 which was previously solved through advanced techniques of characterization (Jiang et al., 2011). Among the proposed set of frameworks, all had the difficulty of being interrupted. Speed up on GPU was the main objective of these initial works. It is worth mentioning here two independent specific computer programs that are related to ZSP, FOCUS (Grosse-Kunstleve et al., 1997, 1999) and Zefsa II (Deem and Newsam, 1989; Deem et al., 1992; Falcioni and Deem, 1999). They are real-space methods specific for zeolite structure solution from powder diffraction data. FOCUS combines automatic Fourier recycling with a zeolitic framework topology search and in the case of Zefsa II, the method of parallel tempering has been advantageously added to the biased Monte Carlo. Our contribution consists on creating a new objective function able to evaluate a viable zeolite

structure and a genetic algorithm hybridized with a heuristic to solve more efficiently the ZSP. Thus, our Parallel Genetic Hybrid Algorithm for Zeolites (P-GHAZ) pursues a double objective: first, to solve more effectively zeolite structures for which the structure elucidation, in the absence of large enough single crystals, needs techniques such as modern electron diffraction that are efficient but heavier and expensive to implement. The second objective consists in generation of thermodynamically stable hypothetical zeolite structures with original topologies.

2. Methods and materials

2.1. Zeolites structure problem

Zeolites are crystalline microporous aluminosilicates for which the pores diameter, according to the nomenclature of IUPAC (McCusker et al., 2001), is less than 20 Å. Their structure results from the assembly of TO_4 tetrahedra ($T = \text{Si}$ and Al), each oxygen atom being common to two tetrahedrons (Fig. 1). Microporosity is ordered and regular, leading to channels and cages distributed periodically in space (Fig. 2). The pores size is of the order of those of conventional molecules and is at the origin of the term “molecular sieve”.

In theory, there is an infinite number of possible zeolitic structures (Treacy et al., 1997, 2004; Delgado et al., 1999) but up to date only 232 zeolitic structures are today recognized by the Structure Commission of the International Zeolite Association (SC-IZA) (Baerlocher and McCusker, 1996). Among them, only 40 are natural. The pore system of a zeolite can be mono- (1D), bi- (2D) or three-dimensional (3D), and each system is designated by its topology. The openings of the channels are generally characterized by the number of T component elements (e.g., 10MR means 10 tetrahedrons rings, or 10-membered ring, as in the case of ZSM-5, a 3D pore system zeolite). After the discovery of a new topology, a three-letter code is assigned by the SC-IZA. This three-letter code is generally linked to the name of the material or the research team responsible for its discovery. For example, the MFI code was assigned to zeolite ZSM-5 (Zeolite Socony Mobil-5 (Five)) (Argauer and Landolt, 1972)

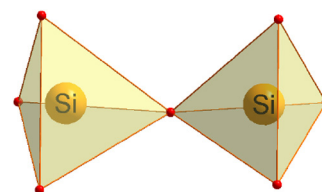


Fig. 1. Two SiO_4 tetrahedrons linked via an oxygen bridge.

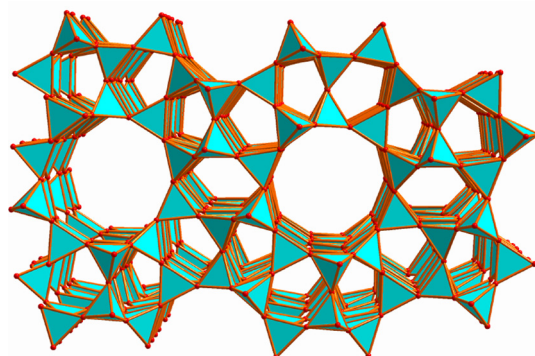


Fig. 2. Structure of zeolite ZSM-5 (Kokotailo et al., 1978) with its medium pores delimited by 10 tetrahedrons.

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