Job offer - Postgraduate research internship:
"Effective metaheuristics for the structural resolution of new zeolites"

- **Duration:** between 3 and 6 months (depending on your constraints)
- **Employer:** University of Haute-Alsace
- **Location:** IRIMAS Institute, Mulhouse, France
- **Indemnities:** Legal amount (around 572 € per month)
- **Supervisors:** Mathieu Brévilliers, Lhassane Idoumghar, Julien Lepagnot, Laurent Moalic, Taylan Ors & Jean-Louis Paillaud

1. Background

Collaboration between the OMEGA team of the IRIMAS Institute of the UHA and the MPC axis of IS2M allowed to progress on the development of a new algorithm dealing with the structural resolution of zeolites. Thus, through this collaboration (one M2 and one thesis), the generation of hypothetical zeolitic structures had led to the generation of original hypothetical structures. The exponential number of potential solutions and the cost of solving this problem make the use of metaheuristics significant for this topic. A new approach based on a parallel hybrid genetic algorithm for zeolites using a modified objective function to find hypothetical zeolitic structures, close to the criterion of thermodynamic feasibility, had been established. A population of random atoms is initialized and at each generation, a crossover operator and a mutation heuristic are applied. Each individual in the population generates a potential zeolitic structure by applying the symmetry operations of a given space group. This structure is evaluated with an objective function. The system, to operate, only needs the lattice parameters, the number of T atoms per elementary lattice and the space group. These three data are generally obtained experimentally.

2. Mission

As an intern, your work will consist in proposing and developing an improved optimization algorithm and objective function, based on the work carried out previously. Since this work is at the interface between the fields of optimization and chemistry of materials, you will discuss with the members of the MPC axis of IS2M to familiarize yourself with the field of application, and to fully understand all aspects of the problem.

3. Required skills

- **Being in the last two years of postgraduate education (in progress) in computer science or applied mathematics.**
- **Very good programming skills.**
- Good optimization / operational research skills.
- Good level of English.

4. Application

To apply, please send an email to julien.lepagnot@uha.fr with the following: **CV, motivation letter, transcripts of grades from the last two years of study**.

5. Bibliography

[1] O. Abdelkafi, L. Idoumghar, J. Lepagnot, J.-L. Paillaud, I. Deroche, L. Baumes & P. Collet, "Using a novel parallel genetic hybrid algorithm to generate and determine new zeolite frameworks", *Computers and Chemical Engineering*, 2017, Vol. 98, pp. 50-60.

[2] O. Abdelkafi, L. Idoumghar, J. Lepagnot & J.-L. Paillaud, "Memory genetic algorithm hybridized for zeolites", *IEEE Congress on Evolutionary Computation*, San Sebastian, Spain, June 2017.

[3] O. Abdelkafi, L. Idoumghar, J. Lepagnot & J.-L. Paillaud, "The determination of new stable zeolite frameworks using a parallel hybrid genetic algorithm", *International Workshop on Optimization and Learning: Challenges and Applications*, Alicante, Spain, February 2018.