

Atomistically informed lattice models for micro-porous materials – size effect in elasticity and fracture properties

Doctoral school	Doctoral School of Exact Sciences and their Applications (↗web-ED211).
University	University Pau and Pays Adour (↗web-UPPA).
Laboratory	Laboratory for the thermodynamics of complex fluids and geological reservoirs UMR5150 UPPA/CNRS/TOTAL (↗web-LFCR).
Research team	Geomechanics and Porous Media (↗web-G2MP).
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Project description: Atomistically informed lattice models for micro-porous materials – size effect in elasticity and fracture properties

Micro-porous materials (with pore sizes under 2nm typically, according to the IUPAC classification) are widely encountered in chemical engineering, oil and gas production, novel material design, manufacturing and pharmaceutical industries, and construction. Zeolites, activated carbon, cement and other construction materials, coal or tight rocks are among these materials. Their mechanical response is of the utmost interest for many practical problems such as the safety analysis of concrete structures or the transitory and long-term responses of geological disposals, where tensile loads and long-term time-dependent deformations may trigger failure.

The major common denominator in these materials is that the physics that govern the material response should be considered at the nanometre scale. As a consequence, continuum based approaches describing the mechanical response of micro-porous materials, which are the only tractable answers to these problems at the engineering scale, ought to be rooted in atomistic-based models in order to provide answers that go beyond a simple phenomenological approach with tuned, macroscopic properties.

This project intends to tackle two related issues: (i) the behaviour of micro-porous materials with high porosity is the result of the mechanical response of pore walls made of a few layers of atoms. Their elastic response is different from that of bulk properties, and size effects on the elastic response of these pore walls are expected; (ii) at such a scale, fracture characteristics ought also to be revisited as they are different from those observed in bulk materials. This is necessary in order to reach a proper description of failure of these materials at the continuum scale. These issues will be tackled by combining atomistic calculations with lattice analyses that represent the material response at the macroscopic scale. Comparisons with a projected experimental campaign to which the doctoral candidate may be associated are also expected.

Candidate's profile

The candidate should hold a master degree in mechanics of materials, applied mechanics (e.g. mechanical engineering or civil engineering). Candidates with profiles dealing with physics of fracture are also welcome. Candidates who are finalizing their master's program and will obtain their master degree in the summer of 2018 are eligible and are strongly encouraged to apply. Previous experience with numerical simulation tools (such as molecular dynamics, finite elements or discrete elements analyses, lattice analysis) is an asset. Proficiency in English is mandatory.

The application procedure is available at: <http://perso.crans.org/gregoire/positions@G2MP>