Intrusion of molecules in zeolites under high pressure: new technology for new materials

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Zeolites are hydrated microporous materials and consist of tetrahedral units – usually Si(Al,P)O₄ – sharing vertices to form a framework characterized by the presence of cages and channels. Thanks to this structural peculiarity, zeolites are considered as nano-molds: a significant part of their structure consists of empty spaces that can be filled by guest molecules.

Purposes of the project

We will exploit the porous template effectiveness of zeolites in inducing aggregation and polymerization along preferential directions. The driving force to promote molecular aggregation and eventually reaction in zeolitic inert molds will be high pressure (HP). The idea of exploiting HP as a tool to obtain confined small-sized supramolecular systems (“hyperconfinement”) is innovative and challenging and will open the way to the synthesis of materials that cannot be obtained in standard conditions. The polymerization of hydrocarbons will be targeted, to give conductive polymers able to be integrated in functional devices, such as gas sensors for environmental purposes.

Aim of the thesis

In the proposed thesis, in situ High Pressure X-Ray Powder Diffraction (HP-XRPD) experiments will be performed by exploiting synchrotron radiation at the beamline BM01@ESRF (Grenoble - France). The experiments will be performed in Diamond Anvil Cell, loaded with the zeolite powder and the hydrocarbons to be polymerized, used as P-transmitting medium.

The collected data will be fitted by Rietveld method and the crystalline structure of the obtained material will be derived.

Additional techniques such as, thermogravimetric analyses, IR and spectroscopy will be exploited in the thesis.

Structure of poly-ethilene polimerized in zeolite silicalite (Santoro et al. 2012, Nature Communications)

Students at work on the beamline during night shift