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HP-induced supra-molecular organization of guest molecules in FER-type zeolites

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The response to pressure of a synthetic all-silica ferrierite (Si-FER) and of a natural ferrierite from Monastir (Sardinia, Italy) (Mon-FER, Na0.56 K1.19 Mg2.02 Ca0.52 Sr0.14)(Al6.89Si29.04)O72 ·17.86 H2O) is here investigated combining HP synchrotron XRPD experiments and molecular dynamics simulations. The experiments were carried out by using penetrating (methanol:ethanol:water 16:3:1, m.e.w.; ethanol:water 1:3, e.w.) and non-penetrating (silicone oil, s.o.) pressure transmitting media (PTM). In Si-FER compressed in e.w., both water (w.) and ethanol molecules (e.) enter the pore system even at 0.2 GPa. The structural refinement of the data collected at 0.8 GPa reveals 8 w. and 4 e. molecules in the 10- and 6-membered ring channels, in tight agreement with the results of MD simulations. In Si-FER compressed at 0.2 GPa in m.e.w., only water molecules penetrate the 10-membered ring channels (15 per u.c.), organized in chains running along the channel axis. The interactions among the guest species and the framework oxygen atoms are very weak, due to the hydrophobicity of the framework. Upon decompression, the intruded extra-molecules are not completely released, so giving rise to new materials with different extra-framework contents. The results obtained for Si-FER compressed in m.e.w. and s.o. were compared to those obtained for Mon-FER, demonstrating that the zeolite composition and the PTM strongly influence the overall elastic parameters of the investigated samples. Specifically, Mon-FER shows a much higher rigidy than Si-FER in both media, due to the stiffening effect of the numerous extraframework species present in the natural sample. The higher rigidity of Si-FER in m.e.w. with respect to s.o. can be explained by the penetration, in the former case, of the PTM molecules, which contribute to stiffen the framework.

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