**Poster Presentation**

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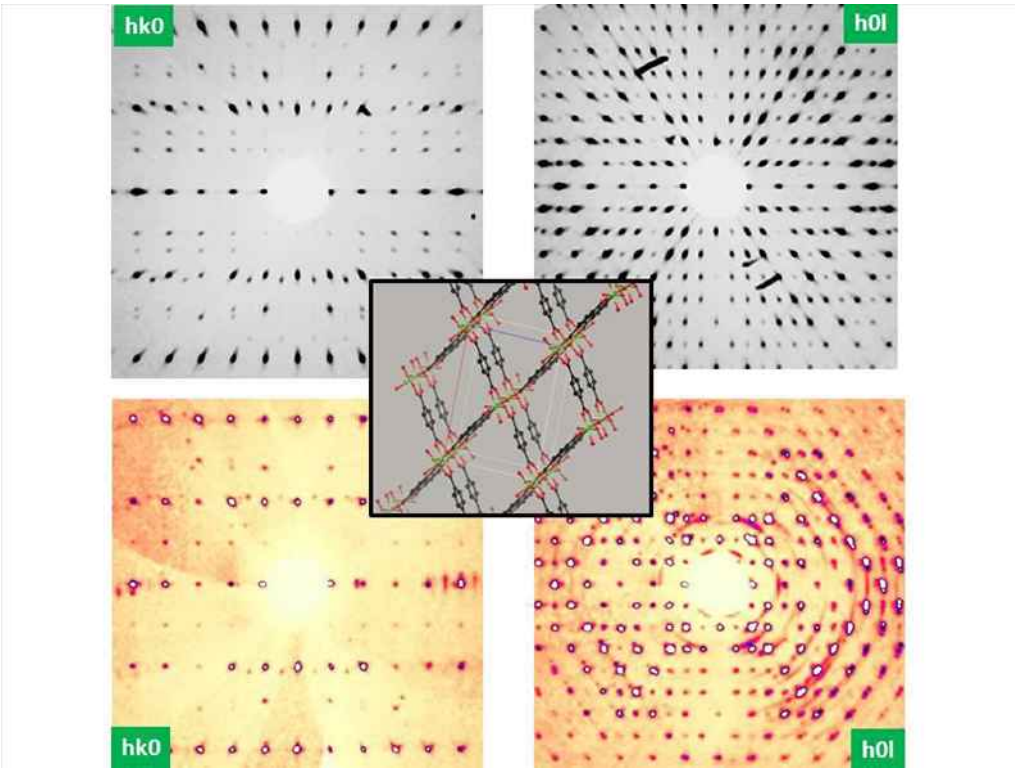
## *X-ray and neutron scattering: from ideal zeolites to real guest-host systems*

F. Porcher[1,2], M. Souhassou[1], C. Lecomte[1]

[1]*CRM2, UMR 7036 CNRS-Université de Lorraine, Vandoeuvre-lès-Nancy, France,* [2]*LLB, UMR 12 CEA-CNRS, Gif-sur-Yvette, France*

Tetrahedral MOFs, microporous metallophosphates and zeolites share common framework topologies despite very different chemical nature of their crystalline skeleton. In the case of zeolites or metallophosphates, the polymeric [TO2]_ framework is based on single tetrahedral atoms T (T= Si4+/Al3+ or Ga3+/B3+/P5+ respectively) connected by corner oxygen atoms O. In the case of MOFs, the skeleton is built from supertetraedra formed by a central metal atom complexed by 4 organic linkers (terephtalate,…); hence homologous structures expanded by a "scale factor". In "molecular sieves", the static porosity but also the "breathing effect" control, in first approximation, the adsorption and the self-diffusion of guest molecules. These latter are finely tuned by the interaction of these molecules with the framework itself (though H-bonds or electrostatic interactions), with charge compensating cations in basic zeolites (through coulombic interaction), or with other adsorbed molecules. However, the interplay between guest molecule adsorption, framework relaxation, cation redistribution and atomic charge transfer leads to an inextricable problem for the modeling and prediction of adsorption properties in these systems in absence of any polarizable and adaptive force field. We will present experimental charge density studies on activated industrial zeolites FAU, MFI and MOR. The electrostatic properties derived on these systems (electric field, atomics charges) are validated by a comparison with those derived, experimentally and theoretically, on a comprehensive set of simpler quartz-type materials (SiO2, AlPO4, GaPO4,…) representative of typical microporous compositions. Finally, we will combine the informations brought by diffraction, diffuse scattering and Monte-Carlo modelling to analyse the adsorption process or the role of the template in the stabilisation of the framework in these systems and in the famous MIL-53 MOF

***[1]*** *E. Borissenko ; F. Porcher ; A. Bouché et al., Microporous Mesoporous Materials, 2008, 114, 155-165,* ***[2]*** *M. Jeffroy; E. Borissenko; A. Boutin et al. Microporous Mesoporous Materials, 2011, 138, 45-50,* ***[3]*** *D. S. Bhange; C. Dejoie; F. Porcher; et al. European Physical Journal, 189, 279-284*

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