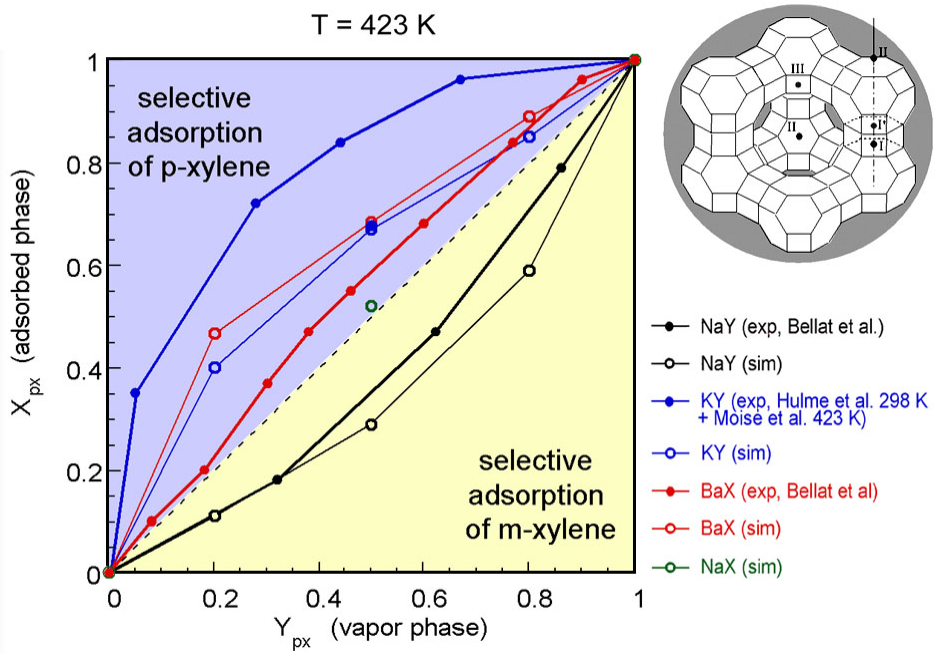
GIBBS

This program computes thermophysical properties of single and multi-phase fluids as well as adsorption isotherms of fluids on solids. The program employs a Gibbs ensemble Monte Carlo method with the interatomic interactions being described by forcefields. The program is the result of a joint development of the French Petroleum Institute and the University of Paris. It is integrated in the MedeA platform with a convenient user interface and analysis tools.



Computed selective adsorption of p-xylene in a zeoltite Y with Na, K, and Ba doping. After Lachet (2001)

Properties from GIBBS

- Thermophysical properties of single phase, multi-component systems
- Equilibria of two-phase systems: liquid-gas and liquid-liquid
- Equilibria of multi-phase systems: liquid-liquid-gas
- Adsorption isotherms of fluids in nanoporous systems such as zeolites

Types of systems

- Rigid, semi-flexible, and flexible linear, branched, and monocyclic molecules
- Molecules with and without charges
- Rigid nanoporous substrates such as zeolites

Required MedeA modules

- Core MedeA environment
- Job Server and Task Servers

More on our website:

www.materialsdesign.com

- MEDEA GIBBS: Liquid - Vapor Pressure Curve of Methane

Relevant Publications

- E Bourasseau, M Haboudou, A Boutin, A Fuchs, and P Ungerer, *J. Chem. Phys.*, vol. 118, no. 7, p. 3020, 2003.
- V Lachet, S Buttefey, A Boutin, and Alain Fuchs, *Physical Chemistry Chemical Physics*, vol. 3, no. 1, p. 80-86, 2001.