Adsorption and Desorption Surface Dynamics of Gaseous Adsorbate on Silicalite-1 by Molecular Dynamics Simulation

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The sticking coefficient is one of the fundamental quantities that quantify the dynamics process at interfaces. It represents the probability that, on approaching the external surface of a particle, a molecule will be captured by the particle and will enter its inner space (for porous solids), rather than being rejected to continue its trajectory in the open space between the particles. The inverse process is quantified by the desorption coefficient. The adsorption/desorption process of different gaseous molecular species on the zeolite silicalite-1 has been investigated using molecular dynamics simulations. Values of the sticking and desorption coefficients were computed for different temperatures and different loadings for ethylene, n-butane, argon, n-heptane [1,2] under equilibrium conditions. The values of the desorption and sticking coefficients will be discussed in relation with the nature of the interaction between the solid and the guest molecules, in particular the adsorption energy and the isotherm of adsorption. These results will give insights in the kinetic process of adsorption and desorption that occurs at the interface between the solid and the gas phase.

References:

[1] J.-M. Simon, J.-B. Bellat, S. Vasenkov, J. Karger. J. Phys. Chem. B **109**, 13523 (2005).
[2] J.-M. Simon, J.-B. Bellat and J. M. Salazar, Mol. Sim. **40**, 52 (2014)