COMPUTERSIMULATION STUDIES OF ZEOLITES AND ALUMINOPHOSPHATES

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Lattice dynamic calculations were performed at elevated temperatures to evaluate the relative stability, crystal structure and thermodynamic properties of zeolites and aluminophosphates.

The approach is based on the Born model of solids in which the forces acting between the atoms are described by interatomic potentials. There have been two major developments in the modelling of these materials. One is the derivation of a reliable potential model for silica and the second is the inclusion of entropic effects in the caleulation of free energies. The calculation of free energies enables us to predict crystal structures and hence thermodynamic properties at elevated temperatures unlike earlier simulations where only properties at zero Kelvin couid be evaluated.

The atomistic simulation methods were used to calculate the relative stability of zeolites with an aim of understanding the factors which govern framework stability. They have been also used to calculate thermodynamic properties like heat capacity and thermal expansion. Especially the calculation of the thermal expansion behaviour has led to an interesting prediction in advance of experiments. Many zeolites and aluminophosphates show a negative coefficient of expansion, which means a contraction of their cell volumes on heating. All results show good agreement with available experimental data, showing the viability of using atomistic simulation to probe the structure and relative stability of zeolites and aluminophosphates.