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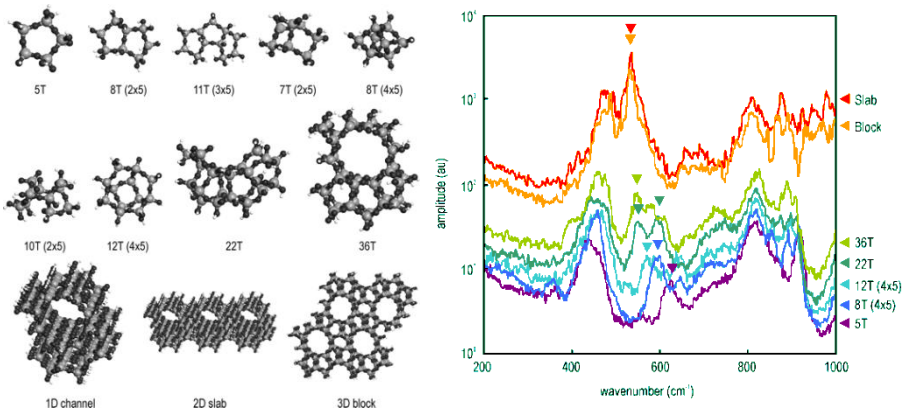
DECOMPOSITION OF VIBRATIONAL SPECTRA OBTAINED WITH MOLECULAR DYNAMICS SIMULATIONS

Keywords: spectroscopy, material characterization, molecular dynamics

The development of new nanoporous materials is a hot research topic given recent advances and successes of this class of novel materials in chemical and pharmaceutical industry. In the quest for innovative materials it is of utmost importance to characterize newly synthesized samples correctly. Conventional experimental techniques for this purpose include Infrared and Raman spectroscopy. These spectra reveal the frequencies of the atomic vibrational modes in the system under study. There is however no one-to-one correspondence between the vibrational frequencies and the structure and composition of a sample.

Molecular dynamics simulations can be used to obtain a simulated spectrum for a given model system. The atomic trajectories can be obtained by integrating the equations of motion of a molecular system contains thousands of atoms when the inter-atomic interactions are modeled with empirical potentials. A Fourier analysis of the atomic velocities can be compared with experimental spectra. Hence it becomes feasible to elucidate the structure of new materials by checking the correspondence between the experimental spectrum and simulated spectra obtained with for a series of model systems. An even more intriguing phenomenon is the evolution of spectra during the synthesis of nanoporous materials. A growth mechanism can then be validated through simulated spectra on all the intermediate crystal precursors. It is also important to correlate topological features with well-defined peaks and bands in the frequency spectrum. Such relations are essential to gain more insight in the evolution of spectra during the synthesis.



Goal A preliminary spectral decomposition method based on molecular dynamics simulations has been developed at the Centre for Molecular Modelling (CMM). Surprising new insights were obtained for small model systems of zeolite clusters. The purpose of this thesis is a generalization of the method for arbitrary molecular topologies. This thesis involves both theoretical developments and the implementation computer codes that perform the decomposition analysis on the output obtained from a molecular dynamics simulation.

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