

## Selective statistical analysis of MD simulations for vibrational spectroscopy modelling

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Infrared and Raman spectroscopy are amongst the most important characterization methods in the domain of nanoscience and nanotechnology. As the analysis of raw data requires careful decomposition of the output signal, modelling plays a crucial role identifying the various physical processes that contribute to the spectrum. The most used *ab initio* modelling techniques like DFT are limited by the computer time required to solve for systems with number of atoms having an order of magnitude of 2 or more.

We present an alternative approach based on the selective statistical analysis of molecular dynamics simulations to model the vibrational spectroscopy of nanostructures. We demonstrate this approach –besides having the obvious advantage regarding the calculation time and system size over *ab initio* methods– is also more relevant and applicable to realistic scenarios especially when one has to deal with systems prone to a lot of parameters like stress, distortion, charging, etc.

We adopt this approach to calculate the radial breathing mode frequencies of cycloparaphenylenes of various sizes and compare our results with DFT values and experimental observations. We also demonstrate a case where the anomaly at Raman response of a carbon nanotube under lateral stress can be successfully elucidated using our approach.