Gauss Fitting of DFT Derived Infrared Spectra

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Infrared Spectroscopy (IR) can help identify chemical substances and active catalytic sites in heterogeneous catalysis through adsorption of probe molecules.[1] Density functional theory (DFT) allows for the simulation of IR spectra of these adsorbed species. In practice, comparing DFT-simulated IR spectra with experimental IR spectra is often cumbersome as DFT data typically only consist of wavenumber and relative intensity of the peaks. Furthermore, a database containing both experimental and simulated spectra data in appropriate formats for easy comparisons does not currently exist. In this contribution, we present a web-based software that can take DFT-simulated IR spectra and replicates the peak broadening of experimental IR spectra by generating Gaussian curves around each peak. The standard deviation can be conveniently adjusted with a slider to match experimental data, which can also be plotted in the same chart.

The software serves as a database adhering to the FAIR (findable, accessible, interoperable, reusable) principles. Additionally, it incorporates specialized analysis and adjustment tools designed for the unique requirements of IR spectroscopy, aiming to enhance workflow efficiency and provide enhanced insights into the generated data.

Figure 1: Comparison between several simulated and experimental IR spectra. Gaussian widening is applied to one of the DFT spectra.