High accuracy *ab initio* rovibrational spectroscopy of non-rigid molecules

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Spectroscopy is the primary tool with which we observe and interrogate small gas-phase molecules. Simulating molecular spectra from first principles requires a combination of high accuracy electronic structure theory and quantum nuclear motion calculations – the latter being the focus of this talk. Although a variety of accurate and efficient methods exist for treating the rotation-vibration dynamics of semi-rigid molecules (i.e. those that undergo only small displacements from their equilibrium geometry), these approaches often fail for non-rigid molecules that exhibit highly anharmonic and large-amplitude nuclear motion. I will discuss some recently developed tools, in particular a rotational extension to curvilinear vibrational Møller-Plesset perturbation theory, that provide accurate spectroscopic parameters – such as vibrational frequencies and rotational constants – for non-rigid molecules of small to medium size. A number of examples, including *gauche*-1,3-butadiene, the simplest conjugated diene, and formamide, the smallest peptide bond-containing molecule, will be used to demonstrate the rich variety of rovibrational dynamics exhibited by non-rigid systems.