# Ab Initio, Post-Harmonic Vibrational Calculations: Bigger and better?

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Progress in the title area has been dramatic over the past ten or so years, as a result of the efforts of many groups. I will review recent work in our group on the two aspects of accurate vibrational calculations, namely accurate potential energy (and dipole moment) surfaces and their use in a variety of VSCF/VCI calculations of vibrational energies and IR spectra. Several recent examples will be presented that illustrate the approaches we have developed in the past ten or so years. They are: potential energy surfaces for the formic acid dimer and nitromethane and 'MULTIMODE' calculations of vibrational energies using them, and many-body, non-covalent interaction potentials for neat water, methane hydrate clathrate, hydrated NaCl and NaF, and 'local monomer' calculations using them. Comparisons with experiment will be made in all the examples presented.

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