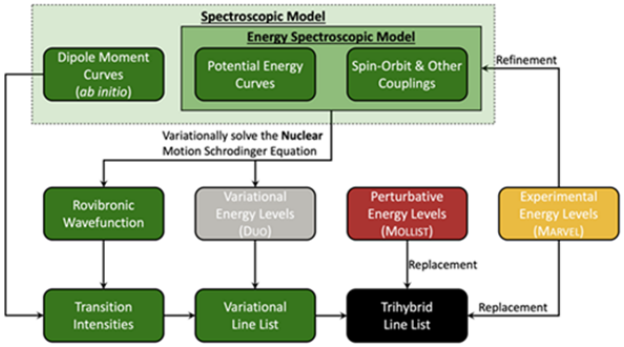
TRIHYBRID LINE LIST CONSTRUCTION FOR NH AND ZrO

ARMANDO N. PERRI, LAURA K McKEMMISH, *School of Chemistry, University of New South Wales, Sydney, NSW, Australia.*

Accurate and comprehensive diatomic molecular spectroscopic data is essential to the measuring and monitoring of gaseous environments, the computational benchmarking of theoretical approaches and, increasingly, in ultracold physics. The recent search for unusual transition metal diatomics, such as TiO and VO, in hot Jupiter exoplanets has demanded spectra of sub 0.1 cm^{-1}accuracy. This experimental need has motivated significant developments in line list construction.



A line list contains the assigned rovibronic energy levels of a molecule, as well as the transition frequencies and intensities between these energy levels. Here, I will discuss the new trihybrid construction of line lists, specifically for NH and ZrO. This trihybrid methodology is advantageous as precedence is given to experimental energy levels that independently form a self-consistent network. This list of energy levels is subsequently interpolated with perturbative calculations using model Hamiltonians and extrapolated with variational calculations using fitted potential energy and coupling curves.

The exemplar cases of NH and ZrO highlight the diversity of electronic structures encountered in line list construction. For NH, only the uncoupled ground and first excited triplet electronic states are considered, as direct transitions to other states are either forbidden or negligible in intensity. Alternatively, for ZrO, eleven highly coupled electronic states are considered as many transitions are allowed and intense, especially in the hot stellar environment of S-type stars that ZrO characterises.