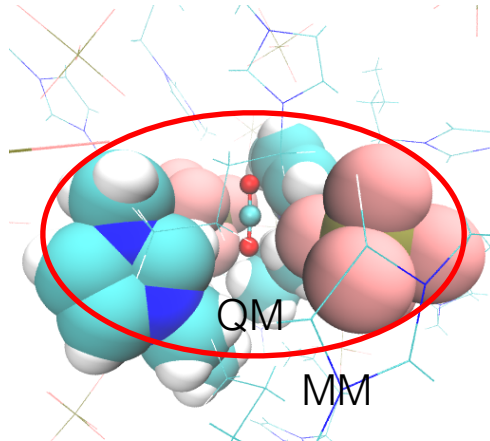
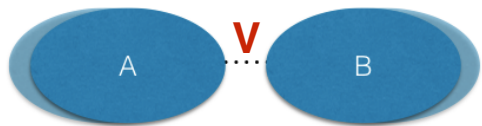


Accurate Anharmonic Frequencies

Solvent Disorder



Energy Decomposition

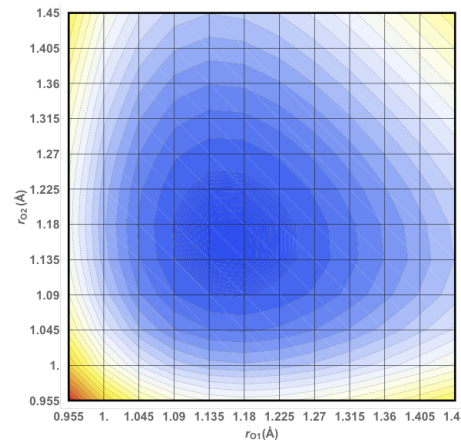
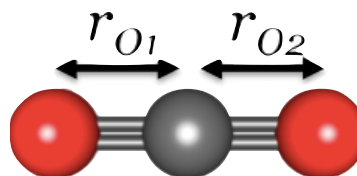


$$H(\zeta, \lambda_A, \lambda_B) = F + \zeta \mathbf{V} + \lambda_A W_A + \lambda_B W_B$$

SAPT

$$[\mathbf{f}_A]_{xx} [\mathbf{T}]_{xx} = [\mathbf{S}_A]_{xx} [\mathbf{T}]_{xx} [\boldsymbol{\varepsilon}]_{xx}$$

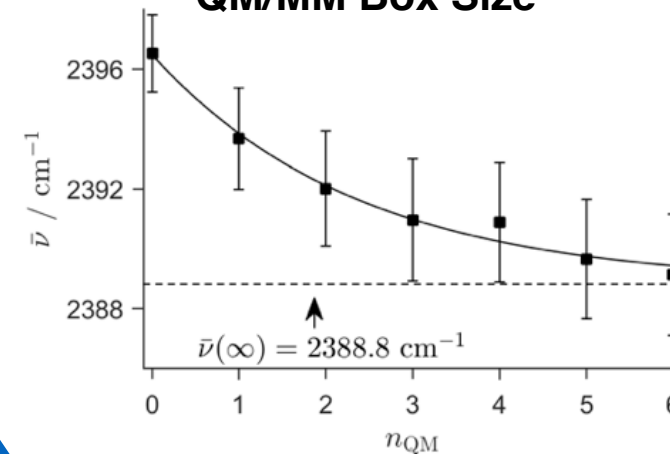
ALMO



$$H = \frac{p_1^2}{2\mu} + \frac{p_2^2}{2\mu} + \frac{p_1 p_2 \cos(\theta)}{m_c} + V(r_1, r_2)$$

Solve Nuclear Quantum Problem via DVR

QM/MM Box Size



Method & Basis Set

