* DMC Subgroup 1-4
  + Ryan- Water in Hexamer
    - 30 GS wavefunctions looking for time step dependence
    - Freeze 5 of hexamer and do DMC of sixth
    - Only 1 of 6 (index 0) displays time step dependence
    - Check for array/algorithm errors
  + Mark
    - Has million walker sim for Nick running
    - Energies look close to Victorss
  + Anne
    - Phase issues in
  + Coire
    - Block out research time
    - Communicate time to Anne and Ryan for accountability
    - Talk to Ryan about doing some of Nicks stuff
  + Fenris
    - New way for computational variance using computer vision
* Group Meeting 1-4
  + Rachel giving practice talk
  + Vibrational coupling in tert-butyl hydrogen peroxide
  + Why?
    - Relevant in atmospheric
  + Has been studied experimentally with spectroscopy
    - Explain spectra
  + Questions
    - Can we develop a simple model
    - What can we learn about the intensity of the combination band from this model?
  + Creating a rediced fimensional model
    - Large molecule
    - Consider which degrees of freedom have the most impact on OH stretch
      * Torsion of CO bond
  + Building model
    - Start with electronic
    - Add adiabatic separations…wut
* Ryan 1/5/21
  + Hyak – Mox- ilahie
    - Priority #1 get set up on the computers
    - #2 rtalk about results once ryan has them
* Subgroup 1/6- Chloe, Rachel, Jacob
  + Jacob
    - Using important sampling and fixed node DMC
    - To get intensity
      * Overlap between first excited and ground state
    - Chart, line chart

      Description automatically generated
    - H3O2-
  + Rachel
* Subgroup 1/11- Ryan, mark, Jacob, Fenris
  + Outline: <https://docs.google.com/document/d/16mpF9tTF4CnrZz-Y33utLQb-1q-jHNisR-jRN9jOQwg/edit>
  + <https://docs.google.com/document/d/1VQOFLGYIoH4MwCeX4CfD_vPLlTGz7Zxak4zq71ScESE/edit>
  + Molecular orbital basis machine learning
  + Pit of despair:
    - Zero-point energy is specific to motion
    - Water would not exist as a liquid if you put in the total ZPE into molecular motion
* Theory Group Meeting
  + Rachel “Huck-mala”
* Group Meeting 1/11- Emil
  + Personal
* Scrum 1/12/2021