

**(1) Molecular dynamics studies of CNN (with Dr Terry Frankcombe)**

The chemistry of nitrogen in interstellar space is highly uncertain, with a large number of poorly characterised reactions contributing. The  $N+CN \rightarrow C+N_2$  reaction is one such reaction. This project involves performing molecular dynamics calculations of  $N+CN$  reactions to explore reaction mechanisms and rates as a function of temperature.

**(2) Molecular potential energy surfaces (PES) for reactions:**

Use ab initio quantum chemistry to construct the PES for interstellar and atmospheric reactions and study the reaction dynamics using computer simulations.

**(3) Molecular energetics of large molecule reactions:**

Calculate the transition states for reactions involving large organic molecules using a method which systematically decomposes the molecules into small clusters of functional groups.