(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 -> C+N2 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.