

Current Interests of the Southampton Electronic Structure Group

John Dyke

1. Calculation of Infrared Frequencies and Intensities of Potential Greenhouse Gases (GHGs) using electronic structure methods.
2. Calculation of Global Warming Potentials (GWPs) of GHGs
3. Calculation of Potential Energy Surfaces of Reactions of Atmospheric Importance using high level electronic structure calculations.
4. Use of these surfaces to calculate reaction rate coefficients and branching ratios using Variational Transition State Theory (VTST).
5. Kinetic studies of reactions of atmospheric importance with a flow-tube, using Photoelectron Spectroscopy (PES) as the detection method

Greenhouse Gas Townhall Meeting Jan 7-8th 2015