

# PUBLICATIONS

Some of the work presented in this thesis has been published in the following papers:

## CHAPTER 2

S. A. Trygubenko and D. J. Wales, *A doubly nudged elastic band method for finding transition states*, J. Chem. Phys. **120**, 2082-2094 (2004).

J. M. Carr, S. A. Trygubenko and D. J. Wales, *Finding pathways between distant local minima*, J. Chem. Phys. **122**, 234903-234910 (2005).

## CHAPTER 3

S. A. Trygubenko and D. J. Wales, *Analysis of cooperativity and localisation for atomic rearrangements*, J. Chem. Phys. **121**, 6689-6697 (2004).

## CHAPTER 4

S. A. Trygubenko and D. J. Wales, *Kinetic analysis of discrete path sampling stationary point databases*, Mol. Phys., in press (2006).