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Publications

Some of the work contained in this thesis has been published in the following papers.

1. Calculation of thermodynamic properties of small Lennard-Jones clusters incorporating anharmonicity, J. P. K. Doye and D. J. Wales, J. Chem. Phys. **102**, 9659–9672 (1995).
2. An order parameter approach to coexistence in atomic clusters, J. P. K. Doye and D. J. Wales, J. Chem. Phys. **102**, 9673–9688 (1995).
3. The effect of the range of the potential on the structures of clusters, J. P. K. Doye, D. J. Wales and R. S. Berry, J. Chem. Phys. **103**, 4234–4249 (1995).
4. Theoretical predictions of structure and thermodynamics in the large cluster regime, D. J. Wales and J. P. K. Doye, in *Large Clusters of Atoms and Molecules (NATO ASI Series E: Vol. 313),* ed. T. P. Martin (Kluwer Academic, Dordrecht, 1996), pp. 241–279.
5. What can calculations employing empirical potentials teach us about bare transition metal clusters?, D. J. Wales, L. J. Munro and J. P. K. Doye, J. Chem. Soc., Dalton Trans. 611–623 (1996).
6. The structure and stability of atomic liquids: from clusters to bulk, J. P. K. Doye and D. J. Wales, Science **271**, 484–487 (1996).
7. The effect of the range of the potential on the structure and stability of simple liquids: from clusters to bulk, from sodium to C_{60}, J. P. K. Doye and D. J. Wales, J. Phys. B **29**, in press (1996). (Invited Review)
8. On potential energy surfaces and relaxation to the global minimum, J. P. K. Doye and D. J. Wales, J. Chem. Phys. **105**, in press (1996).
9. Traversing the potential energy surface by eigenvector-following: applications to global optimisation and the structural transformations of clusters, J. P. K. Doye and D. J. Wales, Z. Phys. D in press.

I have also published the following papers during my PhD.

1. Coexistence and phase separation in clusters: From the small to the not-so-small regime, D. J. Wales and J. P. K. Doye, J. Chem. Phys. **103**, 3061–3070 (1995).
2. Magic numbers and growth sequences of small face-centred-cubic and decahedral clusters, J. P. K. Doye and D. J. Wales, Chem. Phys. Lett. **247**, 339–347 (1995).

3. The structure of $(C_{60})_N$ clusters, J. P. K. Doye and D. J. Wales, Chem. Phys. Lett. in press (1996).
4. Thermally-induced surface reconstructions of Mackay icosahedra, J. P. K. Doye and D. J. Wales, Z. Phys. D in press.