

REFERENCES

- [1] J. Nocedal, *Updating quasi-Newton matrices with limited storage*, Math. Comp. **35**, 773 (1980).
- [2] D. C. Liu and J. Nocedal, *On limited memory BFGS method for large scale optimization*, Math. Prog. **45**, 503 (1989).
- [3] J. Nocedal, *Software for large-scale unconstrained optimization*, <http://www.ece.northwestern.edu/~nocedal/lbfgs.html> (2000).
- [4] B. R. Brooks, R. E. Bruccoleri, B. D. Olafson, D. J. States, S. Swaminathan and M. Karplus, *CHARMM: A program for macromolecular energy, minimization, and dynamics calculations*, J. Comp. Chem. **4**, 187 (1983).
- [5] E. Neria, S. Fischer and M. Karplus, *Simulation of activation free energies in molecular systems*, J. Chem. Phys. **105**, 1902 (1996).
- [6] A. D. Mackerell Jr., D. Bashford, M. Bellott, R. L. D. Jr., J. D. Evanseck, M. J. Field, S. Fischer, J. Gao, H. Guo, S. Ha, D. Joseph-McCarthy, L. Kuchnir, K. Kuczera, F. T. K. Lau, C. Mattos, S. Michnick, T. Ngo, D. T. Nguyen, B. Prodhom, W. E. Reiher III, B. Roux, M. Schlenkrich, J. C. Smith, R. Stote, J. Straub, M. Watanabe, J. Wiorkiewicz-Kuczera, D. Yin and M. Karplus, *All-atom empirical potential for molecular modelling and dynamics studies of proteins*, J. Phys. Chem. B **102**, 3586 (1998).
- [7] S. A. Trygubenko and D. J. Wales, *A doubly nudged elastic band method for finding transition states*, J. Chem. Phys. **120**, 2082 (2004).
- [8] D. J. Wales, *Discrete path sampling*, Mol. Phys. **100**, 3285 (2002).

- [9] D. J. Wales, *Energy landscapes: Applications to clusters, biomolecules and glasses*, Cambridge University Press, Cambridge (2003).
- [10] D. J. Wales, *Some further applications of discrete path sampling to cluster isomerization*, Mol. Phys. **102**, 883 (2004).
- [11] T. Lazaridis and M. Karplus, *Effective energy function for protein dynamics and thermodynamics*, Proteins: Struct., Func. and Gen. **35**, 133 (1999).
- [12] G. M. Crippen and H. A. Scheraga, *Minimization of polypeptide energy. X. A global search algorithm*, Arch. Biochem. Biophys. **144**, 453 (1971).
- [13] J. Pancíř, *Calculation of the least energy path on the energy hypersurface*, Coll. Czech. Chem. Comm. **40**, 1112 (1974).
- [14] R. L. Hilderbrandt, *Application of Newton-Raphson optimization techniques in molecular mechanics calculations*, Comput. Chem **1**, 179 (1977).
- [15] C. J. Cerjan and W. H. Miller, *On finding transition states*, J. Chem. Phys. **75**, 2800 (1981).
- [16] J. Simons, P. Jørgenson, H. Taylor and J. Ozment, *Walking on potential energy surfaces*, J. Phys. Chem. **87**, 2745 (1983).
- [17] A. Banerjee, N. Adams, J. Simons and R. Shepard, *Search for stationary points on surfaces*, J. Phys. Chem. **89**, 52 (1985).
- [18] J. Baker, *An algorithm for the location of transition states*, J. Comp. Chem. **7**, 385 (1986).
- [19] D. J. Wales, *Rearrangements of 55-atom Lennard-Jones and $(C_{60})_{55}$ clusters*, J. Chem. Phys. **101**, 3750 (1994).
- [20] D. J. Wales and J. Uppenbrink, *Rearrangements in model face-centred-cubic solids*, Phys. Rev. B **50**, 12342 (1994).
- [21] L. J. Munro and D. J. Wales, *Rearrangements of bulk face-centred cubic nickel modelled by a Sutton-Chen potential*, Faraday Discuss. **106**, 409 (1997).

- [22] L. J. Munro and D. J. Wales, *Defect migration in crystalline silicon*, Phys. Rev. B **59**, 3969 (1999).
- [23] Y. Kumeda, L. J. Munro and D. J. Wales, *Transition states and rearrangement mechanisms from hybrid eigenvector-following and density functional theory. Application to C₁₀H₁₀ and defect migration in crystalline silicon*, Chem. Phys. Lett. **341**, 185 (2001).
- [24] D. J. Wales and T. R. Walsh, *Theoretical study of the water pentamer*, J. Chem. Phys. **105**, 6957 (1996).
- [25] K. Müller and L. D. Brown, *Location of saddle points and minimum energy paths by a constrained simplex optimization procedure*, Theor. Chim. Acta **53**, 75 (1979).
- [26] M. A. Novotny, *Monte Carlo algorithms with absorbing Markov chains: Fast local algorithms for slow dynamics*, Phys. Rev. Lett. **74**, 1 (1995).
- [27] H. Jónsson, G. Mills and W. Jacobsen, *Nudged elastic band method for finding minimum energy paths of transitions*, in *Classical and quantum dynamics in condensed phase simulations*, edited by B. J. Berne, G. Ciccotti and D. F. Coker, p. 385, World Scientific (1998).
- [28] G. Henkelman and H. Jónsson, *Improved tangent estimate in the nudged elastic band method for finding minimum energy paths and saddle points*, J. Chem. Phys. **113**, 9978 (2000).
- [29] G. Henkelman, B. P. Uberuaga and H. Jónsson, *A climbing image nudged elastic band method for finding saddle points*, J. Chem. Phys. **113**, 9901 (2000).
- [30] G. Henkelman, G. Johannesson and H. Jónsson, *Methods for finding saddle points and minimum energy paths*, in *Progress in theoretical chemistry and physics*, edited by S. D. Schwartz, p. 269, Kluwar Academic Publishers, Dordrecht (2000).
- [31] W. H. Press, B. P. Flannery, S. A. Teukolsky and W. T. Vetterling, *Numerical recipes in Fortran: The art of scientific computing*, Cambridge University Press, Cambridge (1992).

- [32] M. P. Allen and D. J. Tildesley, *Computer simulation of liquids*, Clarendon Press, Oxford (1989).
- [33] Wikipedia, the free encyclopedia, <http://www.wikipedia.org/> (2006).
- [34] J. N. Murrell, S. Carter, S. C. Farantos, P. Huxley and A. J. C. Varandas, *Molecular potential energy functions*, Wiley, Chichester (1984).
- [35] J. N. Murrell, *The many-body expansion of the potential energy function for elemental clusters*, Int. J. Quant. Chem. **37**, 95 (1990).
- [36] R. L. Johnston, *Atomic and molecular clusters*, Taylor & Francis, New York (2002).
- [37] H. B. Schlegel, *Exploring potential energy surfaces for chemical reactions: An overview of some practical methods*, J. Comp. Chem. **24**, 1514 (2003).
- [38] J. N. Murrell and K. J. Laidler, *Symmetries of activated complexes*, Trans. Faraday Soc. **64**, 371 (1968).
- [39] D. J. Wales and J. P. K. Doye, *Stationary points and dynamics in high-dimensional systems*, J. Chem. Phys. **119**, 12409 (2003).
- [40] J. P. K. Doye and D. J. Wales, *Saddle points and dynamics of Lennard-Jones clusters, solids, and supercooled liquids*, J. Chem. Phys. **116**, 3777 (2002).
- [41] F. H. Stillinger, *Exponential multiplicity of inherent structures*, Phys. Rev. E **59**, 48 (1999).
- [42] F. H. Stillinger and T. A. Weber, *Hidden structures in liquids*, Phys. Rev. A **25**, 978 (1982).
- [43] F. H. Stillinger and T. A. Weber, *Packing structures and transitions in liquids and solids*, Science **225**, 983 (1984).
- [44] H. Pelzer and E. Wigner, *The speed constants of the exchange reactions*, Z. Phys. Chem. **B15**, 445 (1932).

- [45] H. Eyring, *The activated complex and the absolute rate of chemical reactions*, Chem. Rev. **17**, 65 (1935).
- [46] M. G. Evans and M. Polanyi, *Some applications of the transition state method to the calculation of reaction velocities, especially in solution*, Trans. Faraday Soc. **31**, 875 (1935).
- [47] W. Forst, *Theory of unimolecular reactions*, Academic Press, New York (1973).
- [48] K. J. Laidler, *Chemical kinetics*, Harper & Row, New York (1987).
- [49] P. Pulay, G. Fogorasi, F. Pang and J. E. Boggs, *Systematic ab initio gradient calculation of molecular geometries, force constants, and dipole moment derivatives*, J. Am. Chem. Soc. **101**, 2550 (1979).
- [50] G. Fogorasi, X. Zhou, P. W. Taylor and P. Pulay, *The calculation of ab initio molecular geometries: efficient optimization by natural internal coordinates and empirical correction by offset forces*, J. Am. Chem. Soc. **114**, 8191 (1992).
- [51] P. Pulay and G. Fogorasi, *Geometry optimization in redundant internal coordinates*, J. Chem. Phys. **96**, 2856 (1996).
- [52] J. Baker, A. Kessi and B. Delley, *The generation and use of delocalized internal coordinates in geometry optimization*, J. Chem. Phys. **105**, 192 (1996).
- [53] C. Peng, P. Y. Ayala, H. B. Schlegel and M. J. Frisch, *Using redundant internal coordinates to optimize equilibrium geometries and transition states*, J. Comp. Chem. **17**, 49 (1996).
- [54] J. Baker, D. Kinghorn and P. Pulay, *Geometry optimization in delocalized internal coordinates: An efficient quadratically scaling algorithm for large molecules*, J. Chem. Phys. **110**, 4986 (1999).
- [55] S. R. Billeter, A. J. Turner and W. Thiel, *Linear scaling geometry optimisation and transition state search in hybrid delocalised internal coordinates*, Phys. Chem. Chem. Phys. **2**, 2177 (2000).

- [56] B. Paizs, J. Baker, S. Suhai and P. Pulay, *Geometry optimization of large biomolecules in redundant internal coordinates*, J. Chem. Phys. **113**, 6566 (2000).
- [57] V. Bakken and T. Helgaker, *The efficient optimization of molecular geometries using redundant internal coordinates*, J. Chem. Phys. **117**, 9160 (2002).
- [58] J. W. McIver and A. Komornicki, *Structure of transition states in organic reactions. General theory and an application to the cyclobutene-butadiene isomerization using a semiempirical molecular orbital method*, J. Am. Chem. Soc. **94**, 2625 (1972).
- [59] D. O'Neal, H. Taylor and J. Simons, *Potential surface walking and reaction paths for C_{2v} $Be + H_2 \leftarrow BeH_2 \rightarrow Be + 2H$ (1A_1)*, J. Phys. Chem. **88**, 1510 (1984).
- [60] S. Bell and J. S. Crighton, *Locating transition states*, J. Chem. Phys. **80**, 2464 (1984).
- [61] D. T. Nguyen and D. A. Case, *On finding stationary states on large-molecule potential energy surfaces*, J. Phys. Chem. **89**, 4020 (1985).
- [62] J. Baker, *An algorithm for geometry optimization without analytical gradients*, J. Comp. Chem. **8**, 563 (1987).
- [63] M. C. Smith, *How to find a saddle point*, Int. J. Quant. Chem. **37**, 773 (1990).
- [64] J. Nichols, H. Taylor, P. Schmidt and J. Simons, *Walking on potential-energy surfaces*, J. Chem. Phys. **92**, 340 (1990).
- [65] J. Baker and W. H. Hehre, *Geometry optimization in Cartesian coordinates: the end of the Z-matrix?*, J. Comp. Chem. **12**, 606 (1991).
- [66] J. Baker, *Geometry optimization in Cartesian coordinates: constrained optimization*, J. Comp. Chem. **13**, 240 (1992).
- [67] C. J. Tsai and K. D. Jordan, *Use of an eigenmode method to locate the stationary points on the potential energy surfaces of selected argon and water clusters*, J. Phys. Chem. **97**, 11227 (1993).

- [68] D. J. Wales, *Locating stationary points for clusters in Cartesian coordinates*, J. Chem. Soc., Faraday Trans. **89**, 1305 (1993).
- [69] S. F. Chekmarev, *A simple gradient method for locating saddles*, Chem. Phys. Lett. **227**, 354 (1994).
- [70] J.-Q. Sun and K. Ruedenberg, *Locating transition states by quadratic image gradient descent on potential energy surfaces*, J. Chem. Phys. **101**, 2157 (1994).
- [71] J.-Q. Sun and K. Ruedenberg, *A simple prediction of approximate transition states on potential energy surfaces*, J. Chem. Phys. **101**, 2168 (1994).
- [72] F. Jensen, *Locating transition structures by mode following: a comparison of six methods on the Ar₈ Lennard-Jones potential*, J. Chem. Phys. **102**, 6706 (1995).
- [73] J. M. Bofill and M. Comajuan, *Analysis of the updated Hessian matrices for locating transition structures*, J. Comp. Chem. **16**, 1326 (1995).
- [74] Q. Zhao and J. B. Nicholas, *Transition state optimization using the divide-and-conquer method: Reaction of trans-2-butene with HF*, J. Chem. Phys. **104**, 767 (1996).
- [75] W. Quapp, *A gradient-only algorithm for tracing a reaction path uphill to the saddle of a potential energy surface*, Chem. Phys. Lett. **253**, 286 (1996).
- [76] J. Baker and F. Chan, *The location of transition states: a comparison of Cartesian, Z-matrix and natural internal coordinates*, J. Comp. Chem. **17**, 888 (1996).
- [77] T. R. Walsh and D. J. Wales, *Rearrangements of the water trimer*, J. Chem. Soc., Faraday Trans. **92**, 2505 (1996).
- [78] P. Y. Ayala and H. B. Schlegel, *A combined method for determining reaction paths, minima, and transition state geometries*, J. Chem. Phys. **107**, 375 (1997).
- [79] A. Ulitsky and D. Shalloway, *Finding transition states using contangency curves*, J. Chem. Phys. **106**, 10099 (1997).

- [80] B. Paizs, G. Fogarasi and P. Pulay, *An efficient direct method for geometry optimization of large molecules in internal coordinates*, J. Chem. Phys. **109**, 6571 (1998).
- [81] O. Farkas and H. B. Schlegel, *Methods for geometry optimization of large molecules. I. An $O(N^2)$ algorithm for solving systems of linear equations for the transformation of coordinates and forces*, J. Chem. Phys. **109**, 7100 (1998).
- [82] N. Mousseau and G. T. Barkema, *Travelling through potential energy landscapes of disordered materials: The activation-relaxation technique*, Phys. Rev. E **57**, 2419 (1998).
- [83] H. Goto, *A frontier mode-following method for mapping saddle points of conformational interconversion in flexible molecules starting from the energy minimum*, Chem. Phys. Lett. **292**, 254 (1998).
- [84] W. Quapp, M. Hirsch, O. Imig and D. Heidrich, *Searching for saddle points of potential energy surfaces by following a reduced gradient*, J. Comp. Chem. **19**, 1087 (1998).
- [85] O. Farkas and H. B. Schlegel, *Methods for optimizing large molecules. II. Quadratic search*, J. Chem. Phys. **111**, 10806 (1999).
- [86] D. J. Wales, J. P. K. Doye, M. A. Miller, P. N. Mortenson and T. R. Walsh, *Energy landscapes: From clusters to biomolecules*, Adv. Chem. Phys. **115**, 1 (2000).
- [87] L. R. Pratt, *A statistical method for identifying transition states in high dimensional problems*, J. Chem. Phys. **85**, 5045 (1986).
- [88] R. Elber and M. Karplus, *A method for determining reaction paths in large molecules: Application to myoglobin*, Chem. Phys. Lett. **139**, 375 (1987).
- [89] R. S. Berry, H. L. Davis and T. L. Beck, *Finding saddles on multidimensional potential surfaces*, Chem. Phys. Lett. **147**, 13 (1988).
- [90] R. Czerminski and R. Elber, *Reaction path study of conformational transitions in flexible systems*, J. Chem. Phys. **92**, 5580 (1990).

- [91] S. Fischer and M. Karplus, *Conjugate peak refinement — an algorithm for finding reaction paths and accurate transition states in systems with many degrees of freedom*, Chem. Phys. Lett. **194**, 252 (1992).
- [92] L. L. Stachó and M. I. Bán, *A global strategy for determining reaction paths. 1. General theory of a procedure finding Fukui intrinsic reaction coordinate*, Theor. Chim. Acta **83**, 433 (1992).
- [93] I. V. Ionova and E. A. Carter, *Ridge method for finding saddle points on potential energy surfaces*, J. Chem. Phys. **98**, 6377 (1993).
- [94] L. L. Stachó and M. I. Bán, *An algorithm for determining dynamically defined reaction paths (DDRP)*, Theor. Chim. Acta **84**, 535 (1993).
- [95] G. Dömöör, M. I. Bán and L. L. Stachó, *Experiences and practical hints on using the DDRP method, illustrated by the example of the H(2)+H reaction*, J. Comput. Chem. **14**, 1491 (1993).
- [96] C. Y. Peng and H. B. Schlegel, *Combining synchronous transit and quasi-Newton methods to find transition states*, Israeli J. Chem. **33**, 449 (1993).
- [97] A. Matro, D. L. Freeman and J. D. Doll, *Locating transition states using double-ended classical trajectories*, J. Chem. Phys. **101**, 10458 (1994).
- [98] O. S. Smart, *A new method to calculate reaction paths for conformational transitions of large molecules*, Chem. Phys. Lett. **222**, 503 (1994).
- [99] M. I. Bán, G. Dömöör and L. L. Stachó, *Dynamically defined reaction-path (DDRP) method*, J. Mol. Struct. (Theochem) **311**, 29 (1994).
- [100] G. Mills and H. Jónsson, *Quantum and thermal effects in H₂ dissociative adsorption: Evaluation of free energy barriers in multidimensional quantum systems*, Phys. Rev. Lett. **72**, 1124 (1994).
- [101] I. V. Ionova and E. A. Carter, *Direct inversion in the iterative subspace-induced acceleration of the ridge method for finding transition states*, J. Chem. Phys. **103**, 5437 (1995).

- [102] L. L. Stachó, G. Dömötör and M. I. Bán, *On the Elber-Karplus reaction path-following method and related procedures*, Chem. Phys. Lett. **311**, 328 (1999).
- [103] R. Elber and M. Karplus, *Reply to a paper by Stachó et al.*, Chem. Phys. Lett. **311**, 335 (1999).
- [104] G. Henkelman and H. Jónsson, *A dimer method for finding saddle points on high dimensional potential surfaces using only first derivatives*, J. Chem. Phys. **111**, 7010 (1999).
- [105] G. Henkelman and H. Jónsson, *Long time scale kinetic Monte Carlo simulations without lattice approximation and predefined event table*, J. Chem. Phys. **115**, 9657 (2001).
- [106] R. A. Miron and K. A. Fichthorn, *The step and slide method for finding saddle points on multidimensional potential surfaces*, J. Chem. Phys. **115**, 8742 (2001).
- [107] P. Maragakis, S. A. Andreev, Y. Brumer, D. R. Reichman and E. Kaxiras, *Adaptive nudged elastic band approach for transition state calculation*, J. Chem. Phys. **117**, 4651 (2002).
- [108] L. Xie, H. Liu, and W. Yang, *Adapting the nudged elastic band method for determining minimum-energy paths of chemical reactions in enzymes*, J. Chem. Phys. **120**, 8039 (2004).
- [109] B. Peters, A. Heyden, A. T. Bell and A. Chakraborty, *A growing string method for determining transition states: Comparison to the nudged elastic band and string methods*, J. Chem. Phys. **120**, 7877 (2004).
- [110] R. Crehuet and M. J. Field, *A temperature-dependent nudged elastic band algorithm*, J. Chem. Phys. **118**, 9563 (2003).
- [111] M. E. J. Newman, *The structure and function of complex networks*, SIAM Review **45**, 167 (2003).
- [112] R. S. Berry and R. Breitengraser-Kunz, *Topography and dynamics of multidimensional interatomic potential surfaces*, Phys. Rev. Lett. **74**, 3951 (1995).

- [113] M. A. Miller, J. P. K. Doye and D. J. Wales, *Structural relaxation in atomic clusters: Master equation dynamics*, Phys. Rev. E **60**, 3701 (1999).
- [114] J. P. K. Doye and D. J. Wales, *Structural transitions and global minima of sodium chloride clusters*, Phys. Rev. B **59**, 2292 (1999).
- [115] J. P. K. Doye and C. P. Massen, *Characterizing the network topology of the energy landscapes of atomic clusters*, J. Chem. Phys. **122**, 084105 (2005).
- [116] S. H. Strogatz, *Exploring complex networks*, Nature **410**, 268 (2001).
- [117] D. J. Watts and S. H. Strogatz, *Collective dynamics of ‘small-world’ networks*, Nature **393**, 440 (1998).
- [118] A. L. Barabási and R. Albert, *Emergence of scaling in random networks*, Science **286**, 509 (1999).
- [119] J. S. Andrade, H. J. Herrmann, R. F. S. Andrade and L. R. da Silva, *Apollonian networks: Simultaneously scale-free, small world, Euclidean, space filling, and with matching graphs*, Phys. Rev. Lett. **94**, 018702 (2005).
- [120] E. Nelson, *Dynamical theories of Brownian motion*, Princeton University Press, Princeton (1967).
- [121] H. C. Berg, *Random walks in biology*, Princeton University Press, Princeton (1993).
- [122] W. Forst, *Unimolecular reactions: A concise introduction*, Cambridge University Press, Cambridge (2003).
- [123] G. R. Grimmett and D. R. Stirzaker, *Probability and random processes*, Oxford University Press, Oxford (2005).
- [124] I. Todhunter, *History of the mathematical theory of probability*, Cambridge University Press, Cambridge (1965).
- [125] T. A. Halgren and W. N. Lipscomb, *The synchronous-transit method for determining reaction pathways and locating molecular transition states*, Chem. Phys. Lett. **49**, 225 (1977).

- [126] M. J. S. Dewar, E. F. Healy and J. J. P. Stewart, *Location of transition states in reaction mechanisms*, J. Chem. Soc., Faraday Trans. 2 **80**, 227 (1984).
- [127] C. Cardenas-Lailhacar and M. C. Zerner, *Searching for transition-states — the line-then-plane (LTP) approach*, Int. J. Quant. Chem. **55**, 429 (1995).
- [128] D. A. Liotard, *Algorithmic tools in the study of semiempirical potential surfaces*, Int. J. Quant. Chem. **44**, 723 (1992).
- [129] C. Choi and R. Elber, *Reaction path study of helix formation in tetrapeptides — effect of side chains*, J. Chem. Phys. **94**, 751 (1991).
- [130] F. Jensen, *Introduction to computational chemistry*, John Wiley & Sons (1999).
- [131] CSEP, *Electronic book on mathematical optimization*, <http://csep1.phy.ornl.gov/mo/mo.html> (1995).
- [132] R. Fletcher, *Practical methods of optimization*, John Wiley & Sons (2001).
- [133] D. A. Evans and D. J. Wales, *The free energy landscape and dynamics of met-enkephalin*, J. Chem. Phys. **119**, 9947 (2003).
- [134] H. Goldstein, *Classical mechanics*, Addison-Wesley, Reading, Massachusetts (1980).
- [135] F. S. Acton, *Numerical methods that work*, Mathematical Association of America, Washington (1990).
- [136] D. R. Alfonso and K. D. Jordan, *A flexible nudged elastic band program for optimisation of minimum energy pathways using ab initio electronic structure methods*, J. Comp. Chem. **24**, 990 (2003).
- [137] D. R. Alfonso, *Driver for performing minimum energy path optimizations using the nudged elastic band algorithm*, <http://www.pitt.edu/~alfonso/NEB/neb.html> (2002).
- [138] D. J. Wales, *OPTIM: A program for optimizing geometries and calculating reaction pathways*, <http://www-wales.ch.cam.ac.uk/OPTIM/> (2006).

- [139] M. P. Hodges, *Xmakemol: A program for visualizing atomic and molecular systems, version 5.14*, <http://www.nongnu.org/xmakemol/> (2006).
- [140] *Mathematica, version 5.0*, Wolfram Research, Inc., Champaign, Illinois (1996).
- [141] D. J. Wales, *A Mathematica notebook containing some simple programs for making and manipulating triangulated polyhedra*, <http://www-wales.ch.cam.ac.uk/software.html> (2002).
- [142] Y. M. Rhee, *Construction of an accurate potential energy surface by interpolation with Cartesian weighting coordinates*, *J. Chem. Phys.* **113**, 6021 (2000).
- [143] C. Eckart, *Some studies concerning rotating axes and polyatomic molecules*, *Phys. Rev.* **47**, 552558 (1935).
- [144] A. D. McLachlan, *A mathematical procedure for superimposing atomic coordinates of proteins*, *Acta. Crystallogr. A* **28**, 656 (1972).
- [145] A. Y. Dymarsky and K. N. Kudin, *Computation of the pseudorotation matrix to satisfy the Eckart axis conditions*, *J. Chem. Phys.* **122**, 124103 (2005).
- [146] M. Dierksen, *Comment on “Computation of the pseudorotation matrix to satisfy the Eckart axis conditions”*, *J. Chem. Phys.* **122**, 227101 (2005).
- [147] A. Y. Dymarsky and K. N. Kudin, *Response to “Comment on ‘Computation of the pseudorotation matrix to satisfy the Eckart axis conditions’ ”*, *J. Chem. Phys.* **122**, 227102 (2005).
- [148] R. E. Leone and P. von R. Schleyer, *Degenerate carbonium ions*, *Angew. Chem. Int. Ed. Engl.* **9**, 860 (1970).
- [149] J. P. K. Doye, M. A. Miller and D. J. Wales, *Evolution of the potential energy surface with size for Lennard-Jones clusters*, *J. Chem. Phys.* **111**, 8417 (1999).
- [150] J. P. Neirotti, F. Calvo, D. L. Freeman and J. D. Doll, *Phase changes in 38-atom Lennard-Jones clusters. I. A parallel tempering study in the canonical ensemble*, *J. Chem. Phys.* **112**, 10340 (2000).

- [151] F. Calvo, J. P. Neirotti, D. L. Freeman and J. D. Doll, *Phase changes in 38-atom Lennard-Jones clusters. II. A parallel tempering study of equilibrium and dynamic properties in the molecular dynamics and microcanonical ensembles*, J. Chem. Phys. **112**, 10350 (2000).
- [152] F. H. Stillinger and T. A. Weber, *Dynamics of structural transitions in liquids*, Phys. Rev. A **28**, 2408 (1983).
- [153] E. W. Dijkstra, *A note on two problems in connection with graphs*, Numerische Math. **1**, 269 (1959).
- [154] T. H. Cormen, C. E. Leiserson, R. L. Rivest and C. Stein, *Introduction to algorithms*, The MIT Press, Cambridge, Massachusetts , Cambridge, Mass., 2nd edn. (2001).
- [155] E. W. Weisstein, ‘*Complete graph*’. From Mathworld — A Wolfram web resource, <http://mathworld.wolfram.com/CompleteGraph.html> (2005).
- [156] A. G. Cochran, N. J. Skelton and M. A. Starovasnik, *Tryptophan zippers: Stable, monomeric β -hairpins*, Proc. Natl. Acad. Sci. USA **98**, 5578 (2001).
- [157] C. D. Snow, L. Qiu, D. Du, F. Gai, S. J. Hagen and V. S. Pande, *Trp zipper folding kinetics by molecular dynamics and temperature-jump spectroscopy*, Proc. Natl. Acad. Sci. USA **101**, 4077 (2004).
- [158] D. Du, Y. Zhu, C. Huang and F. Gai, *Understanding the key factors that control the rate of β -hairpin folding*, Proc. Natl. Acad. Sci. USA **101**, 15915 (2004).
- [159] J. D. Bloom, *Computer simulations of protein aggregation*, Master’s thesis, University of Cambridge (July 2002).
- [160] H. M. Berman, J. Westbrook, Z. Feng, G. Gilliland, T. N. Bhat, H. Weissig, I. N. Shindyalov and P. E. Bourne, *The protein data bank*, Nucleic Acids Research **28**, 235 (2000).
- [161] Z. Li and H. A. Scheraga, *Structure and free energy of complex thermodynamic systems*, Proc. Natl. Acad. Sci. USA **84**, 6611 (1987).

- [162] D. J. Wales and J. P. K. Doye, *Global optimization by basin-hopping and the lowest energy structures of Lennard-Jones clusters containing up to 110 atoms*, J. Phys. Chem. A. **101**, 5111 (1997).
- [163] D. J. Wales and H. A. Scheraga, *Global optimization of clusters, crystals and biomolecules*, Science **285**, 1368 (1999).
- [164] C. Branden and J. Tooze, *Introduction to protein structure*, Taylor & Francis, New York (1999).
- [165] S. A. Trygubenko, *Rotamers in CHARMM19 force field*, <http://www.trygub.com/charmm/rotamers/> (2006).
- [166] R. Koradi, M. Billeter and K. Wüthrich, *MOLMOL: A program for display and analysis of macromolecular structures*, J. Mol. Graphics **14**, 51 (1996).
- [167] J. M. Carr, S. A. Trygubenko and D. J. Wales, *Finding pathways between distant local minima*, J. Chem. Phys. **122**, 234903 (2005).
- [168] J. P. K. Doye and D. J. Wales, *Calculation of thermodynamic properties of small Lennard-Jones clusters incorporating anharmonicity*, J. Chem. Phys. **102**, 9659 (1995).
- [169] F. Calvo, J. P. K. Doye and D. J. Wales, *Quantum partition functions from classical distributions: Application to rare-gas clusters*, J. Chem. Phys. **114**, 7312 (2001).
- [170] P. G. Mezey, *Catchment region partitioning of energy hypersurfaces. I.*, Theor. Chim. Acta **58**, 309 (1981).
- [171] T. F. Middleton and D. J. Wales, *Energy landscapes of some model glass formers*, Phys. Rev. B **64**, 24205 (2001).
- [172] S. Sastry, P. G. Debenedetti and F. H. Stillinger, *Signatures of distinct dynamical regimes in the energy landscape of a glass-forming liquid*, Nature **393**, 554 (1998).
- [173] S. D. Stoddard and J. Ford, *Numerical experiments on the stochastic behavior of a Lennard-Jones gas system*, Phys. Rev. A **8**, 1504 (1973).

- [174] M. Vogel, B. Doliwa, A. Heuer and S. C. Glotzer, *Particle rearrangements during transitions between local minima of the potential energy landscape of a binary Lennard-Jones liquid*, J. Chem. Phys. **120**, 4404 (2004).
- [175] M. Arndt, R. Stannarius, H. Groothues, E. Hempel and F. Kremer, *Length scale of cooperativity in the dynamic glass transition*, Phys. Rev. Lett. **79**, 2077 (1997).
- [176] L. Berthier, *Time and length scales in supercooled liquids*, Phys. Rev. E **69**, 20201 (2004).
- [177] D. J. Wales, *A microscopic basis for the global appearance of energy landscapes*, Science **293**, 2013 (2001).
- [178] T. V. Bogdan and D. J. Wales, *New results for phase transitions from catastrophe theory*, J. Chem. Phys. **120**, 11090 (2004).
- [179] M. G. Bulmer, *Principles of statistics*, Dover Publications, New York (1979).
- [180] K. D. Ball, R. S. Berry, R. E. Kunz, F. Y. Li, A. Proykova and D. J. Wales, *From topographies to dynamics on multidimensional potential energy surfaces of atomic clusters*, Science **271**, 963 (1996).
- [181] S. A. Trygubenko, *Rearrangements of LJ₇₅ cluster localized on two atoms*, <http://www.trygub.com/ExtremeRearrangement/LJ75/2atom.html> (2006).
- [182] Y. Gebremichael, M. Vogel and S. C. Glotzer, *Particle dynamics and the development of string-like motion in a simulated monoatomic supercooled liquid*, J. Chem. Phys. **120**, 4415 (2004).
- [183] T. S. Jain and J. J. de Pablo, *Influence of confinement on the vibrational density of states and the boson peak in a polymer glass*, J. Chem. Phys. **120**, 9371 (2004).
- [184] T. F. Middleton and D. J. Wales, *Energy landscapes of model glasses. II. Results for constant pressure*, J. Chem. Phys. **118**, 4583 (2003).
- [185] B. Doliwa and A. Heuer, *Energy barriers and activated dynamics in a supercooled Lennard-Jones liquid*, Phys. Rev. E **67**, 031506 (2003).

- [186] A. Saksengwijit, B. Doliwa and A. Heuer, *Description of the dynamics in complex energy landscapes via metabasins: A simple model study*, J. Phys. Cond. Matt. **15**, S1237 (2003).
- [187] G. Bolch, S. Greiner, H. de Meer and K. S. Trivedi, *Queueing networks and Markov chains*, John Wiley and Sons, New York (1998).
- [188] G. R. Grimmett and D. R. Stirzaker, *One thousand exercises in probability*, Oxford University Press, Oxford (2005).
- [189] N. G. van Kampen, *Stochastic processes in physics and chemistry*, Elsevier, Amsterdam (1981).
- [190] A. B. Bortz, M. H. Kalos and J. L. Lebowitz, *A new algorithm for Monte Carlo simulation of Ising spin systems*, J. Comput. Phys. **17**, 10 (1975).
- [191] K. A. Fichthorn and W. H. Weinberg, *Theoretical foundations of dynamical Monte Carlo simulations*, J. Chem. Phys **95**, 1090 (1991).
- [192] M. A. Miller, *Energy landscapes and dynamics of model clusters*, Ph.D. thesis, University of Cambridge (March 1999).
- [193] M. Block, R. Kunert, E. Schöll, T. Boeck and T. Teubner, *Kinetic Monte Carlo simulation of formation of microstructures in liquid droplets*, New J. Phys. **6**, 166 (2004).
- [194] D. Mukherjee, C. G. Sonwane and M. R. Zachariah, *Kinetic Monte Carlo simulation of the effect of coalescence energy release on the size and shape evolution of nanoparticles grown as an aerosol*, J. Chem. Phys. **119**, 3391 (2003).
- [195] F. M. Bulnes, V. D. Pereyra and J. L. Riccardo, *Collective surface diffusion: n-fold way kinetic Monte Carlo simulation*, Phys. Rev. E **58**, 8692 (1998).
- [196] R. E. Kunz, *Dynamics of first-order phase transitions*, Deutsch, Thun (1995).
- [197] D. A. Evans and D. J. Wales, *Folding of the GB1 hairpin peptide from discrete path sampling*, J. Chem. Phys. **121**, 1080 (2004).

- [198] M. S. Apaydin, D. L. Brutlag, C. Guestrin, D. Hsu and J.-C. Latombe, *Stochastic roadmap simulation: An efficient representation and algorithm for analyzing molecular motion*, in *Recomb '02: Proceedings of the sixth annual international conference on computational biology*, pp. 12–21. ACM Press, New York, NY (2002).
- [199] M. S. Apaydin, C. E. Guestrin, C. Varma, D. L. Brutlag and J.-C. Latombe, *Stochastic roadmap simulation for the study of ligand-protein interactions*, Bioinf. **18**, S18 (2002).
- [200] N. Singhal, C. D. Snow and V. S. Pande, *Using path sampling to build better Markovian state models: Predicting the folding rate and mechanism of a tryptophan zipper beta hairpin*, J. Chem. Phys. **121**, 415 (2004).
- [201] G. Chartrand, *Introductory graph theory*, Dover Publications, New York (1977).
- [202] NIST, *Dictionary of algorithms and data structures*, <http://www.nist.gov/dads/> (2005).
- [203] A. Bar-Haim and J. Klafter, *On mean residence and first-passage times in finite one-dimensional systems*, J. Chem. Phys. **109**, 5187 (1998).
- [204] B. E. Trumbo, *Relationship between the Poisson and exponential distributions*, <http://www.sci.csuhayward.edu/statistics/Resources/Essays/PoisExp.htm> (1999).
- [205] T. F. Middleton, *Energy landscapes of model glasses*, Ph.D. thesis, University of Cambridge (March 2003).
- [206] D. A. Reed and G. Ehrlich, *Surface diffusivity and the time correlation of concentration fluctuations*, Surf. Sci. **105**, 603 (1981).
- [207] A. F. Voter, *Introduction to the kinetic Monte Carlo method*, in *Radiation effects in solids*, pp. 1–22. Springer-Verlag, New York (2005).
- [208] I. Goldhirsch and Y. Gefen, *Analytic method for calculating properties of random walks on networks*, Phys. Rev. A **33**, 2583 (1986).

- [209] I. Goldhirsch and Y. Gefen, *Biased random walk on networks*, Phys. Rev. A **35**, 1317 (1987).
- [210] M. Raykin, *First-passage probability of a random walk on a disordered one-dimensional lattice*, J. Phys. A **26**, 449 (1992).
- [211] K. P. N. Murthy and K. W. Kehr, *Mean first-passage time of random walks on a random lattice*, Phys. Rev. A **40**, 2082 (1989).
- [212] G. H. Weiss, *First-passage time problems in chemical physics*, Adv. Chem. Phys. **13**, 1 (1967).
- [213] W. Ledermann and G. E. H. Reuter, *Spectral theory for the differential equations of simple birth and death processes*, Philos. T. Roy. Soc. A **A246**, 321 (1954).
- [214] S. Karlin and J. L. MacGregor, *The differential equations of birth and death processes*, Trans. Am. Math. Soc. **85**, 489 (1957).
- [215] C. W. Gardiner, *Handbook of stochastic methods in physics, chemistry and the natural sciences*, Springer, Berlin (1985).
- [216] C. V. den Broeck, *A glimpse into the world of random walks*, in *Proceedings of NATO conference on noise and nonlinear phenomena in nuclear systems*, edited by J. L. Munoz-Cobo and F. C. Difilippo, pp. 3–18. Plenum, New York (1988).
- [217] P. L. Doussal, *First-passage time for random walks in random environments*, Phys. Rev. Lett. **62**, 3097 (1989).
- [218] K. P. N. Murthy and K. W. Kehr, *Erratum: Mean first-passage time of random walks on a random lattice*, Phys. Rev. A **41**, 1160 (1990).
- [219] O. Matan and S. Havlin, *Mean first-passage time on loopless aggregates*, Phys. Rev. A **40**, 6573 (1989).
- [220] P. A. Pury and M. O. Cáceres, *Mean first-passage and residence times of random walks on asymmetric disordered chains*, J. Phys. A **36**, 2695 (2003).
- [221] M. Slutsky, M. Kardar and L. A. Mirny, *Diffusion in correlated random potentials, with applications to DNA*, Phys. Rev. E **69**, 061903 (2004).

- [222] M. Slutsky and L. A. Mirny, *Kinetics of protein-DNA interaction: Facilitated target location in sequence-dependent potential*, Biophys. J. **87**, 4021 (2004).
- [223] Ya. G. Sinai, *The limiting behaviour of a one-dimensional random walk in random environment*, Theor. Prob. and Appl. **27**, 256 (1982).
- [224] H. E. Stanley and S. Havlin, *Generalisation of the Sinai anomalous diffusion law*, J. Phys. A **20**, L615 (1987).
- [225] R. D. Vale and R. A. Milligan, *The way things move: Looking under the hood of molecular motor proteins*, Science **288**, 88 (2000).
- [226] R. D. Astumian, *Thermodynamics and kinetics of a Brownian motor*, Science **276**, 917 (1997).
- [227] P. G. de Gennes, *Problems of DNA entry into a cell*, Physica A **274**, 1 (1999).
- [228] A. Meller, L. Nivon and D. Branton, *Voltage-driven DNA translocations through a nanopore*, Phys. Rev. Lett. **86**, 3435 (2001).
- [229] K. Mussawisade, J. E. Santos and G. M. Schütz, *Branching-annihilating random walks in one dimension: Some exact results*, J. Phys. A **31**, 4381 (1998).
- [230] C. Sire, *Analytical results for random walks in the presence of disorder and traps*, Phys. Rev. E **60**, 1464 (1999).
- [231] M. F. Schlesinger and J. Klafter, *Random walks in liquids*, J. Phys. Chem. **93**, 7023 (1989).
- [232] I. Herbut and S. Milosevic, *Hopping on hierarchical structures and random walking on deterministic fractals*, J. Phys. A **23**, 99 (1990).
- [233] L. Acedo and S. B. Yuste, *Territory covered by N random walkers on fractal media: The Sierpinski gasket and the percolation aggregate*, Phys. Rev. E **63**, 011105 (2000).
- [234] M. Bauer, D. Bernard and J. M. Luck, *Even-visiting random walks: exact and asymptotic results in one dimension*, J. Phys. A **34**, 2659 (2001).

- [235] V. I. Alkhimov, *The problem of a self-avoiding random walk*, Uspekhi Fizicheskikh Nauk **161**, 133 (1991).
- [236] I. Majid, D. Ben-Avraham, S. Havlin and H. E. Stanley, *Exact-enumeration approach to random walks on percolation clusters in two dimensions*, Phys. Rev. B **30**, 1626 (1984).
- [237] B. L. Trus, S. Havlin and D. Stauffer, *Distribution of first-passage times for diffusion at the percolation threshold*, J. Phys. A **20**, 6627 (1987).
- [238] E. W. Montroll and G. H. Weiss, *Random walks on lattices. II.*, J. Math. Phys. **6**, 167 (1965).
- [239] J. M. Luck, *A numerical study of diffusion and conduction in a 2D random medium*, J. Phys. A **17**, 2069 (1984).
- [240] D. Zheng, Y. Liu and Z. D. Wang, *Matrix method for random walks on lattices*, J. Phys. A **28**, L409 (1995).
- [241] H. M. Taylor and S. Karlin, *An introduction to stochastic modeling*, Academic Press, New York (1998).
- [242] S. Goldberg, *Probability: An introduction*, Dover Publications, New York (1960).
- [243] B. Kahng and S. Redner, *Scaling of the first-passage time and the survival probability on exact and quasi-exact self-similar structures*, J. Phys. A **22**, 887 (1989).
- [244] S. K. Kim and H. H. Lee, *Crystallinity and average grain size of films grown by chemical vapor deposition*, J. Appl. Phys. **78**, 3809 (1995).
- [245] P. C. Bressloff, V. M. Dwyer and M. J. Kearney, *A ‘sum-over-paths’ approach to diffusion on trees*, J. Phys. A **29**, 1881 (1996).
- [246] S. Revathi, V. Balakrishnan, S. Lakshmibala and K. P. N. Murthy, *Validity of the mean-field approximation for diffusion on a random comb*, Phys. Rev. E **54**, 2298 (1996).
- [247] K. Kim, J. S. Choi and Y. S. Kong, *Multifractals of normalized first passage time in Sierpinski gasket*, J. Phys. Soc. Jpn. **67**, 1583 (1998).

- [248] K. Kim, G. H. Kim and Y. S. Kong, *Multifractal measures characterized by the iterative map with two control parameters*, Fractals **8**, 181 (2000).
- [249] J. Asikainen, J. Heinonen and T. Ala-Nissila, *Exact and efficient discrete random walk method for time-dependent two-dimensional environments*, Phys. Rev. E **66**, 066706 (2002).
- [250] D. ben Avraham, S. Redner and Z. Cheng, *Random walk in a random multiplicative environment*, J. Stat. Phys. **56**, 437 (1989).
- [251] Y. Gefen and I. Goldhirsch, *The building blocks of random walks*, Physica D **38**, 119 (1989).
- [252] H. Haucke, S. Washburn, A. D. Benoit, C. P. Umbach and R. A. Webb, *Universal scaling of nonlocal and local resistance fluctuations in small wires*, Phys. Rev. B **41**, 12454 (1990).
- [253] S. Revathi and V. Balakrishnan, *Diffusion coefficient for random walks on strips with spatially inhomogeneous boundaries*, J. Phys. A **26**, 467 (1993).
- [254] S. H. Noskowicz and I. Goldhirsch, *First-passage-time distribution in a random random walk*, Phys. Rev. A **42**, 2047 (1990).
- [255] S. Revathi and V. Balakrishnan, *Analytic calculation of the diffusion coefficient for random walks on strips of finite width — dependence on size and nature of boundaries*, Phys. Rev. E **47**, 916 (1993).
- [256] V. Balakrishnan and C. Vandenbroeck, *Transport properties on a random comb*, Physica A **217**, 1 (1995).
- [257] A. R. Kerstein and R. B. Pandey, *Conductivity exponent for stirred superconductor-insulator mixtures*, Phys. Rev. B **35**, 3575 (1987).
- [258] Y. Gefen and I. Goldhirsch, *Relation between the classical resistance of inhomogeneous networks and diffusion*, Phys. Rev. B **35**, 8639 (1987).
- [259] Y. Gefen and I. Goldhirsch, *Biased diffusion on random networks: mean first-passage time and DC conductivity*, J. Phys. A **18**, L1037 (1985).

- [260] J. W. Haus and K. W. Kehr, *Diffusion in regular and disordered lattices*, Phys. Reports **150**, 263 (1987).
- [261] I. G. S. H. Noskowicz, *Distribution functions for random walk processes on networks: An analytic method*, J. Stat. Phys. **48**, 255 (1987).
- [262] R. Landauer and M. Buttiker, *Diffusive traversal time — effective area in magnetically induced interference*, Phys. Rev. B **36**, 6255 (1987).
- [263] R. Tao, *Studies of the spectral dimension for branched Koch curves*, J. Phys. A **20**, 6151 (1987).
- [264] J. Koplik, S. Redner and D. Wilkinson, *Transport and dispersion in random networks with percolation disorder*, Phys. Rev. A **37**, 2619 (1988).
- [265] N. M. van Dijk, *Queueing networks and product forms*, John Wiley and Sons, New York (1993).
- [266] E. Gelenbe and G. Pujolle, *Introduction to queueing networks*, John Wiley and Sons, New York (1998).
- [267] A. E. Conway and N. D. Georganas, *Queueing networks - exact computational algorithms*, The MIT Press, Cambridge, Massachusetts (1989).
- [268] D. Eppstein, Z. Galil and G. F. Italiano, *Dynamic graph algorithms*, in *Algorithms and theory of computation handbook*, edited by M. J. Atallah, chap. 8, CRC Press (1999).
- [269] B. V. Cherkassky, A. V. Goldberg and T. Radzik, *Shortest paths algorithms: Theory and experimental evaluation*, in *Soda '94: Proceedings of the fifth annual ACM-SIAM symposium on discrete algorithms*, pp. 516–525, Society for Industrial and Applied Mathematics, Philadelphia, PA (1994).
- [270] G. Ramalingam and T. Reps, *An incremental algorithm for a generalization of the shortest-path problem*, J. Algorithms **21**, 267 (1996).
- [271] G. Ramalingam and T. Reps, *On the computational complexity of dynamic graph problems*, Theor. Comput. Sci. **158**, 233 (1996).

- [272] S. A. Trygubenko and D. J. Wales, *Kinetic analysis of discrete path sampling stationary point databases*, Mol. Phys., in press (2006).
- [273] *GNU general public license*, <http://www.gnu.org/copyleft/gpl.html> (2006).
- [274] S. A. Trygubenko, *Graph transformation program*, <http://www.trygub.com/gt/> (2006).
- [275] *Debian — the universal operating system*, <http://www.debian.org/> (2006).
- [276] M. L. Fredman and R. E. Tarjan, *Fibonacci heaps and their uses in improved network optimisation algorithms*, Journal of the ACM **34**, 596 (1987).
- [277] J. Pitman, *Probability*, Springer-Verlag, New York (1993).
- [278] N. A. Weiss, *A course in probability*, Pearson, Addison Wesley, Boston (2006).
- [279] P. Labastie and R. L. Whetten, *Statistical mechanics of the cluster solid-liquid transition*, Phys. Rev. Lett. **65**, 1567 (1990).
- [280] R. S. Berry, T. L. Beck, H. L. Davis and J. Jellinek, *Solid-liquid phase behavior in microclusters*, Adv. Chem. Phys. **70B**, 75 (1988).
- [281] P. Chen, *A random walk or color chaos on the stock market? Time-frequency analysis of S&P indexes*, Stud. in Nonlin. Dyn. and Econ. **1**, 87 (1996).
- [282] M. J. Plank and B. D. Sleeman, *A reinforced random walk model of tumour angiogenesis and anti-angiogenic strategies*, Math. Med. Bio. **20**, 135 (2003).
- [283] W. E, W. Ren and E. Vanden-Eijnden, *String method for the study of rare events*, Phys. Rev. B **66**, 052301 (2002).
- [284] W. E, W. Ren and E. Vanden-Eijnden, *Energy landscape and thermally activated switching of submicron-sized ferromagnetic elements*, J. Appl. Phys. **93**, 2275 (2003).
- [285] W. Quapp, *Reaction pathways and projection operators: Application to string methods*, J. Comp. Chem. **25**, 1277 (2004).

- [286] W. E, W. Ren and E. Vanden-Eijnden, *Finite temperature string method for the study of rare events*, J. Phys. Chem. A. **109**, 6688 (2005).
- [287] W. Ren, E. Vanden-Eijnden, P. Maragakis and W. E, *Transition pathways in complex systems: Application of the finite-temperature string method to the alanine dipeptide*, J. Chem. Phys. **123**, 134109 (2005).
- [288] W. Quapp, *A growing string method for the reaction pathway defined by a Newton trajectory*, J. Chem. Phys. **122**, 174106 (2005).
- [289] J. W. Chu, B. L. Trout and B. R. Brooks, *A super-linear minimization scheme for the nudged elastic band method*, J. Chem. Phys. **119**, 12708 (2003).
- [290] D. A. Evans, *Energy landscapes and dynamics of model peptides*, Ph.D. thesis, University of Cambridge (December 2003).
- [291] J. M. Carr, *Energy landscapes and dynamics of model proteins*, Ph.D. thesis, University of Cambridge (April 2005).
- [292] R. E. Bellman, *On a routing problem*, Quat. Appl. Math **16**, 87 (1958).
- [293] L. R. Ford and D. R. Fulkerson, *Flows in networks*, Princeton University Press, Princeton (1962).
- [294] E. F. Moore, *The shortest path through a maze*, in *Proceedings of the international symposium on the theory of switching*, pp. 285–292. Harvard University Press, Harvard (1959).