References

1. D.M. Hirst, *A Computational Approach to Chemistry* (Blackwell Scientific Publications, Oxford, 1990)
2. Numerical recipes (http://www.nr.com/oldverswitcher.html)
3. M.S. Child, *Semiclassical Mechanics with Molecular Applications* (Oxford Press Inc., New York, 2005)
4. E. Garcia, A. Laganà, Diatomic potential functions for triatomic scattering. Mol. Phys. **56**, 621–627 (1985)
5. C.J. Joachain, *Quantum Collision Theory* (North-Holland Physics Publishing, Amsterdam, 1975)
6. S. Brandt, H.D. Dahmen, *The Picture Book of Quantum Mechanics* (Wiley, New York, 1985)
7. L. Landau, E. Lifshitz, *Physical-Theoretical Mechanics* (Editori Riuniti, Rome, 1976)
8. N.F. Mott, H.S.W. Massey, *The Theory of Atomic Collisions* (Oxford University Press, Oxford, 1965)
9. M. Abramowitz, I.A. Stegun, *Handbook of Mathematical Functions: With Formulas, Graphs, and Mathematical Tables* (Dover Publications, New York, 2010)
10. A. Schawlow, T.W. Hnsch, G.W. Series, The spectrum of atomic hydrogen. Sci. Am. **240**, 94 (1979)
11. I.N. Levine, *Quantum Chemistry* (Prentice-Hall Inc., New Jersey, 1991)
12. R.G. Newton, *Theory of Scattering Waves and Particles* (McGraw-Hill Book Company, New York, 1966)
13. S. Flügge, *Practical Quantum Mechanics* (Springer, New York, 1970)
14. R. McWeeny, *Methods of Molecular Quantum Mechanics*, 2nd edn. (Academic Press, London, 1992)
15. F. Jensen, *Introduction to Computational Chemistry*, 2nd edn. (Wiley, New York, 2007)
16. B.M. Rode, T.S. Hofer, M.D. Kugler, *The basic of Theoretical and Computational Chemistry* (Wiley-Vch GMBH, New York, 2007). ISBN 978-3-527-31773-8
17. Quantum Chemistry packages list: http://en.wikipedia.org/wiki/List_of_quantum_chemistry_and_solid_state_physics_software
18. W.K. Hastings, Monte Carlo sampling methods using Markov chains and their application. Biometrika **57**(1), 97 (1970)
19. M. Caffarel, P. Claverie, J. Chem. Phys. **88**(2), 1088 (1988)
20. A. Szabo, N.S. Ostlund, *Modern Quantum Chemistry: Introduction to Advanced Electronic Structure Theory* (Dover Publications, New York, 1996)
21. C.C.J. Roothaan, New developments in molecular orbital theory. Rev. Mod. Phys. **23**, 69–89 (1951)

A. Laganà and G. A. Parker (eds.), *Chemical Reactions*, Theoretical Chemistry and Computational Modelling, https://doi.org/10.1007/978-3-319-62356-6

22. B. Roos, Chem. Phys. Lett. **15**, 153 (1972)
23. W.J. Hehre, L. Radom, P. von R. Schleyer, J.A. Pople, *Ab Initio Molecular Orbital Theory* (Wiley, New York, 1986)
24. P.J. Kuntz, E.M. Nemeth, J.C. Polanyi, S.D. Rosner, C.E. Young, J. Chem. Phys. **44**, 1168 (1966)
25. G.C. Schatz, Fitting potential energy surfaces, in *Reaction and Molecular Dynamics*, Lecture Notes in Chemistry, ed. by A. Laganà, A. Riganelli (Springer, Berlin, 2000), p. 15
26. J.N. Murrell, S. Carter, S.C. Farantos, P. Huxley, A.J.C. Varandas, *Molecular Potential Energy Functions* (Wiley, Chichester, 1984)
27. E. Garcia, A. Laganà, A new bond order functional form for triatomic molecules: a fit of the BeFH potential energy. Mol. Phys. **56**, 629–639 (1985)
28. A. Aguado, M. Paniagua, J. Chem. Phys. **96**, 1265 (1992)
29. B.J. Braams, J.M. Bowman, Permutationally invariant potential energy surfaces in high dimensionality. Int. Rev. Phys. Chem. **28**, 4 (2009)
30. K.C. Thompson, M.A. Collins, J. Chem. Soc. Faraday Trans. **93**, 871 (1997)
31. P. Lancaster, K. Salkauskas, *Curve and Surface Fitting: An Introduction* (Academic, London, 1986)
32. P.J. Kuntz, in *Atom Molecule Collision Theory*, ed. by R.B. Bernstein (Plenum, New York, 1979), p. 79
33. A.J.C. Varandas, A.I. Voronin, Mol. Phys. **85**, 497 (1995)
34. E. Garcia, C. Sanchez, A. Rodriguez, A. Lagana, A MEP-MPE potential energy surface for the Cl + CH4 reaction. Int. J. Quantum Chem. **106**, 623–630 (2006)
35. A. Laganà, A rotating bond order formulation of the atom diatom potential energy surface. J. Chem. Phys. **95**, 2216–2217 (1991)
36. M. Verdicchio, Atmospheric reentry calculations and extension of the formats of quantum chemistry data to quantum dynamics, Master Thesis, University of Perugia, 2009
37. D. Wang, J.R. Stallcop, W.M. Huo, C.E. Dateo, D.W. Schwenke, H. Partridge, J. Chem. Phys. **118**, 2186–2189 (2003)
38. B.R.L. Galvão, A.J.C. Varandas, J. Phys. Chem. A **113**, 14424–14430 (2009)
39. A. Laganà, E. Garcia, J. Chem. Phys. **103**, 5410 (1995)
40. S. Rampino, J. Phys. Chem. A **120**(27), 4683–4692 (2016)
41. T.W. Hansch, A.L. Schawlow, G.W. Series, The spectrum of atomic hydrogen. Sci. Am. **240**, 94 (1979)
42. T.J. Zielinski, E. Harvey, R. Sweeney, D.M. Hanson, Quantum states of atoms and molecules. J. Chem. Educ. **82**(12), 1880 (2005)
43. R.J. Bartlett, M. Musial, Coupled-cluster theory in quantum chemistry. Rev. Mod. Phys. **79**, 91 (2007)
44. H.D. Meyer, F. Gatti, G.A. Worth, in *Multidimensional Quantum Dynamics: MCTDH Theory and Applications*, ed. by H.D. Meyer, F. Gatti, G.A. Worth (Wiley, Chichester, 2009)
45. D. Skouteris, A. Laganà, in, Lecture Notes in Computer Science **6784**, 442–452 (2011)
46. D. Skouteris, J.F. Castillo, D.E. Manolopulos, ABC: a quantum reactive scattering program. Comp. Phys. Commun. **133**, 128135 (2000)
47. D. Skouteris, D. Pacifici, L. Laganà, Time dependent wavepacket calculations for the $N(^4S)$ + $N_2(^1\Sigma_g^+)$ system on a LEPS surface: inelastic and reactive probabilities. Mol. Phys. **102**(21–22), 2237–2248 (2004)
48. M. Hankel, M. Smith, C. Sean, S.K. Gray, G.G. Balint-Kurti, DIFFREALWAVE: a parallel real wavepacket code for the quantum mechanical calculation of reactive state-to-state differential cross sections in atom plus diatom collisions. Comput. Phys. Commun. **179**(8), 569–578 (2008)
49. R.T. Pack, G.A. Parker, J. Chem. Phys. **87**, 3888 (1987)
50. U. Manthe, in *Direct calculations of reaction rates in Reaction and Molecular Dynamics*, ed. by A. Laganà, A. Riganelli (Springer, Berlin, 2000), p. 130
51. M. Beck, A. Jakle, G. Worth, H.D. Meyer, The multiconfiguration time dependent Hartree (MCTDH) method: a highly efficient algorithm for propagating wavepackets. Phys. Rep. **324**, 15 (2000)

52. G.G. Balint-Kurti, Time dependent quantum approaches to chemical reactivity, in *Reaction and Molecular Dynmics*, ed. by A. Laganà, A. Riganelli (Springer, Berlin, 2000), p. 74; G.G. Balint-Kurti, A. Palov, *Theory of Molecular collisions*, (Royal Society of Chemistry, 2015)
53. J.C. Light, T. Carrington, Adv. Chem. Phys. **114**, 263 (2000)
54. J. Crawford, G.A. Parker, State-to-state three-atom time-dependent reactive scattering in hyperspherical coordinates. J. Chem. Phys. **138**, 054313 (2013). A version of the code is available for distribution
55. D. Chase, Phys. Rev. **104**, 838 (1956)
56. R.T. Pack, J. Chem. Phys. **60**, 653 (1974)
57. T. Kato, On the adiabatic theorem of quantum mechanics. J. Phys. Soc. Jpn. **5**(6), 435439 (1950)
58. J.M. Bowman, Approximate time independent methods for polyatomic reactions, in Lecture Notes in Chemistry, ed. by A. Laganà, A. Riganelli (Springer, Berlin, 2000), p. 101
59. J.R. Schmidt, P.V. Parandekar, J.C. Tully, Mixed quantum-classical equilibrium: surface hopping. J. Chem. Phys. **129**, 044104 (2008)
60. A. Abedi, N.T. Maitra, E.K.U. Gross, Phys. Rev. Lett. **105**, 123002 (2010)
61. W.H. Miller, The semiclassical initial value representation: a potentially practical way for adding quantum effects to classical molecular dynamics simulations. J. Phys. Chem. A **105**, 2942–2955 (2001)
62. H. Jeffreys, Proc. Lond. Math. Soc. **23**, 428 (1925)
63. G. Wentzel, Z. Phys. **38**, 518 (1926)
64. H.A. Kramers, Z. Phys. **39**, 828 (1926)
65. L. Brillouin, J. Phys. **7**, 353 (1926)
66. R.A. Marcus, Chem. Phys. Lett. **7**, 525 (1970)
67. L. Ciccarelli, E. Garcia, A. Laganà, A quantum mechanical test of the DIM surface of the Li + HCl semi-empirical surface. Chem. Phys. Lett. **120**, 75–79 (1985)
68. D.R. Herschbach, Y.T. Lee, J.C. Polanyi, Nobel lecture december 8, 1986, from Nobel lectures, in *Chemistry 1981-1990*, ed. by T. Frängsmyr, B.G. Malmström (World Scientific Publishing Co., Singapore, 1992)
69. G.C. Schatz, A. Kuppermann, Quantum mechanical scattering for three dimensional atom plus diatom systems: II accurate cross sections for H + H_2. J. Chem. Phys. **66**, 4668 (1977)
70. A. Laganà, N. Faginas Lago, R. Gargano, P.R.P. Barreto, On the semiclassical initial value calculation of thermal rate coefficients for the N + N2 reaction. J. Chem. Phys. **125**, 114311–114317 (2006)
71. A. Bar-Nun, A. Lifshitz, J. Chem. Phys. **47**, 2878 (1967)
72. R.A. Back, J.Y.P. Mui, J. Phys. Chem. **66**, 1362 (1962)
73. R. Lyon, Can. J. Chem. **50**, 1437 (1972)
74. D. Skouteris, O. Gervasi, A. Laganà, Non-Born-Oppenheimer MCTDH calculations on the confined H_2^+ molecular ion. Chem. Phys. Lett. **500**(1–3), 144–148 (2010)
75. http://www.molcas.org/
76. http://www.molpro.net/
77. M.W. Schmidt, K.K. Baldridge, J.A. Boatz, S.T. Elbert, M.S. Gordon, J.H. Jensen, S. Koseki, N. Matsunaga, K.A. Nguyen, S. Su, T.L. Windus, M. Dupuis, J.A. Montgomery, J. Comput. Chem. **14**, 1347 (1993), GAMESS-US see http://www.msg.ameslab.gov/gamess/
78. http://www.gaussian.com/
79. M. Valiev, E.J. Bylaska, N. Govind, K. Kowalski, T.P. Straatsma, H.J.J. van Dam, D. Wang, J. Nieplocha, E. Apra, T.L. Windus, W.A. de Jong, NWChem: a comprehensive and scalable open-source solution for large scale molecular simulations. Comput. Phys. Commun. **181**, 1477 (2010), http://www.nwchem-sw.org/index.php/Main_Page
80. R. Ahlrichs, M. Bar, M. Haser, H. Horn, C. Kolmel, Electronic structure calculations on workstation computers: the program system Turbomole. Chem. Phys. Lett. **162**(3), 165–169 (1989)
81. F. Neese, The ORCA program system. WIREs Comput. Mol. Sci. **2**, 7378 (2012)
82. http://www.hondoplus.com/

83. R.D. Amos, J.E. Rice, *CADPAC, The Cambridge Analytical Derivatives Package* (Cambridge, England, 1987), http://www-theor.ch.cam.ac.uk/software/cadpac.html
84. D. Cappelletti, F. Pirani, B. Bussery-Honvault, L. Gomez, M. Bartolomei, A bond-bond description of the intermolecular interaction energy: the case of weakly bound N_2H_2 and N_2N_2 complexes. Phys. Chem. Chem. Phys. **10**(29), 4281–4293 (2008)
85. F. Pirani, D. Cappelletti, G. Liuti, Range, strength and anisotropy of intermolecular forces in atom-molecule systems: an atom-bond pairwise additivity approach. Chem. Phys. Lett. **350**(3), 286–296 (2001)
86. A. Laganà, A bond order approach to a process oriented fitting of potential energy surfaces. VIRT&L-COMM.10.2016.2
87. F. Pirani, S. Brizi, L.F. Roncaratti, P. Casavecchia, D. Cappelletti, F. Vecchiocattivi, Beyond the Lennard-Jones model: a simple and accurate potential function probed by high resolution scattering data useful for molecular dynamics simulations. Phys. Chem. Chem. Phys. **10**(36), 5489–503 (2008)
88. A. Laganà, G. Ochoa de Aspuru, E. Garcia, J. Phys. Chem. **99**, 17139 (1995)
89. G. Ochoa de Aspuru, D.C. Clary, New potential energy function for four-atom reactions. Application to OH + H_2. J. Phys. Chem. **102**(47), 96319637 (1998)
90. A. van der Avoird, P.E.S. Wormer, A.P.J. Jansen, J. Chem. Phys. **84**, 1629–1635 (1986)
91. J.R. Stallcop, H. Partridge, Chem. Phys. Lett. **281**, 212–220 (1997)
92. D. Capelletti, F. Vecchiocattivi, F. Pirani, E.L. Heck, A.S. Dickinson, Mol. Phys. **93**, 485–499 (1988)
93. V. Aquilanti, M. Bartolomei, D. Cappelletti, E. Carmona-Novillo, F. Pirani, J. Chem. Phys. **117**, 615–627 (2002)
94. L. Gomez, B. Bussery-Honvault, T. Cauchy, M. Bartolomei, D. Cappelletti, F. Pirani, Chem. Phys. Lett. **445**, 99–107 (2007)
95. R. Hellmann, Mol. Phys. **111**, 387–401 (2013)
96. D. Cappelletti, F. Pirani, B. Bussery-Honvault, L. Gomez, M. Bartolomei, Phys. Chem. Chem. Phys. **10**, 4281–4293 (2008)
97. L. Pacifici, M. Verdicchio, N. Faginas Lago, A. Lombardi, A. Costantini, J. Comput. Chem. **34**, 2668–2676 (2013)
98. Y. Paukku, K.R. Yang, Z. Varga, D.G. Truhlar, J. Chem. Phys. **139**, 044309 (2013)
99. Y. Paukku, K.R. Yang, Z. Varga, D.G. Truhlar, J. Chem. Phys. **140**, 019903 (2014)
100. J.D. Bender, S. Doraiswamy, D.G. Truhlar, G.V. Candler, J. Chem. Phys. **140**, 054302 (2014)
101. N. Parsons, D.A. Levin, A.C.T. van Duin, T. Zhu, J. Chem. Phys. **141**, 234307 (2014)
102. J.D. Bender, P. Valentini, I. Nompelis, Y. Paukku, Z. Varga, D.G. Truhlar, T. Schwartzentruber, G.V. Candler, J. Chem. Phys. **143**, 054304 (2015)
103. http://www.giss.nasa.gov/tools/molscat/
104. G.D. Billing, Chem. Phys. Lett. **76**, 178 (1980)
105. M. Cacciatore, A. Kurnosov, A. Napartovich, J. Chem. Phys. **123**, 174315 (2005)
106. E. Garcia, A. Laganà, F. Pirani, M. Bartolomei, M. Cacciatore, A. Kurnosov, On the efficiency of collisional $O_2 + N_2$ vibrational energy exchange. J. Phys. Chem. B **120**, 1476–1485 (2016)
107. S. Rampino, N. Faginas Lago, A. Laganà, F. Huarte-Larrañaga, An extension of the grid empowered molecular simulator GEMS to quantum reactive scattering. J. Comput. Chem. **33**, 708714 (2012)
108. A. Laganà, E. Garcia, A. Paladini, P. Casavecchia, N. Balucani, The last mile of molecular reaction dynamics virtual experiments: the case of the OH(N=1−10)+CO(j= 0−3) reaction. Faraday Discuss. Chem. Soc. **157**, 415–436 (2012)
109. L. Verlet, Computer experiments on classical fluids. Phys. Rev. **159**, 98 (1967)
110. W.L. Hase, R.J. Duchovic, X. Hu, A. Komornicki, K.F. Lim, D. Lu, G.H. Peslherbe, K.N. Swamy, S.R. van de Linde, A.J.C. Varandas, H. Wang, R.J. Wolf, Chemical dynamics software and simulation system (CDSSIM system). QCPE Bull. **16**, 43 (1996), https://cdssim.chem.ttu.edu/nav/htmlpages/licensemenu.jsp
111. M. Ceotto, S. Atahan, S. Shin, First principles semiclassical initial value representation molecular dynamics. Phys. Chem. Chem. Phys. **11**, 3861–3867 (2009)

112. W. Smith, T.R. Forester, DL_POLY2 a general purpose parallel molecular dynamics simulation package. J. Mol. Graph. **14**(3), 136–141 (1996)
113. S. Pronk, S. Pll, R. Schulz, P. Larsson, P. Bjelkmar, R. Apostolov, M. Shirts, J. Smith, P. Kasson, D. van der Spoel, B. Hess, E. Lindahl, GROMACS 4.5: a high-throughput and highly parallel open source molecular simulation toolkit. Bioinformatics **29**(7), 845–854 (2013)
114. J.C. Phillips, R. Braun, W. Wang, J. Gumbart, E. Tajkhorshid, E. Villa, C. Chipot, R.D. Skeel, L. Kale, K. Schulten, Scalable molecular dynamics with NAMD. J. Comput. Chem. **26**, 1781 (2005)
115. O. Trott, A.J. Olson, AutoDock Vina: improving the speed and accuracy of docking with a new scoring function, efficient optimization and multithreading. J. Comput. Chem. **31**, 455 (2010)
116. CADDSuite, http://www.ballview.org/caddsuite
117. Flexx, http://www.biosolveit.de/FlexX/
118. K.J. Bowers, E. Chow, H. Xu, R.O. Dror, M.P. Eastwood, B.A. Gregersen, J.L. Klepeis, I. Kolossvry, M.A. Moraes, F.D. Sacerdoti, J.K. Salmon, Y. Shan, D.E. Shaw, Scalable algorithms for molecular dynamics simulations on commodity clusters, in *Proceedings of the ACM/IEEE Conference on Supercomputing (SC06)* (IEEE, New York, 2006)
119. W.D. Cornell, P. Cieplak, C.I. Bayly, I.R. Gould, K.M. Merz Jr., D.M. Ferguson, D.C. Spellmeyer, T. Fox, J.W. Caldwell, P.A. Kollman, A second generation force field for the simulation of proteins, nucleic acids, and organic molecules. J. Am. Chem. Soc. **117**, 5179 (1995)
120. S. Dietrich, I. Boyd, Scalar and parallel optimized implementation of the direct simulation Monte Carlo method. J. Comput. Phys. **126**, 328 (1996)
121. G.A. Bird, *Molecular Gas Dynamics* (Clarendon, Oxford, 1976)
122. G.A. Bird, *Molecular Gas Dynamics and the Direct Simulation of Gas Flows* (Claredon, Oxford, 1994)
123. H.S. Tsein, Superaerodynamics, mechanics of rarefied gases. J. Aerosp. Sci. **13**, 342 (1946)
124. C.-D. Munz, M. Auweter-Kurtz, S. Fasoulas et al., Coupled particle-in-cell and direct simulation Monte Carlo method for simulating reactive plasma flows. Comptes Rendus Mecanique **342**(10–11), 662 (2014)
125. The European Grid Initiative (EGI), http://www.egi.eu/infrastructure. Accessed 19 Feb 2015
126. https://wiki.egi.eu/wiki/VT_Towards_a_CMMST_VRC
127. A. Voss, R. Procter, Virtual research environments in scholarly work and communications. Libr. Hi Tech **27**(2), 174 (2009)
128. A. Laganà, A. Riganelli, O. Gervasi, On the structuring of the Computational Chemistry Virtual Organization COMCPHEM, Lecture Notes in Computer Science (2006), pp. 665–674
129. A. Laganà, DRAG: a cluster of spinoffs for grid and cloud services. VIRT&L-COMM.5.2014.16
130. A. Capriccioli, Report on PROGEO progress. VIRT&L-COMM.8.2015.2
131. A. Laganà, The Molecular science community for open science. VIRT&L-COMM.9.2016.6
132. A. Laganà, C. Manuali, L. Pacifici, S. Rampino, A new bottom up approach to the CMMST VRE. VIRT&L-COMM.7.2015.8
133. A. Laganà, Research and innovative actions. Chemistry, molecular and material science and technologies virtual research environment (CMMST-VRE). VIRT&L-COMM.6.2014.1
134. C. Manuali, A. Laganà, Requirements of the chemistry, molecular and materials sciences and technologies community for evaluating the quality of a service. VIRT&L-COMM.5.2014.14
135. C. Manuali, A. Laganà, Trial user, resources and services quality evaluation for grid communities sustainability, Lecture Notes in Computer Science (2015), p. 324
136. J. Crawford, G.A. Parker, State-to-state three-atom time-dependent reactive scattering in hyperspherical coordinates. J. Chem. Phys. **138**, 054313 (2013)
137. X. Li, G.A. Parker, Theory of laser enhancement of ultra-cold reactions: The Fermion-Boson population transfer adiabatic passage of $^{6}Li + {}^{6}Li^{7}Li(Tr=1mK) \rightarrow {}^{6}Li_2 + {}^{7}Li(Tp=1mK)$. J. Chem. Phys. **128**, 184113 (2008)

138. X. Li, G.A. Parker, P. Brumer, I. Thanopulos, M. Shapiro, Theory of laser enhancement and suppression of cold reactions: the Fermion-Boson $^6Li + {}^7Li_2 \rightarrow {}^6Li^7Li + {}^7Li$ radiative collision. J. Chem. Phys. **128**, 124314 (2008)
139. X. Li, G.A. Parker, P. Brumer, I. Thanopulos, M. Shapiro, Laser-catalyzed production of ultracold molecules: the $^6Li + {}^6Li^7Li \rightarrow {}^7Li + {}^6Li_2$ reaction. Phys. Rev. Lett. **101**, 043003 (2008)
140. X. Li, D.A. Brue, G.A. Parker, New method for calculating bound states: the A1 states of Li_3 on the spin-aligned ($^4A''$) potential surface. J. Chem. Phys. **127**, 014108 (2007)
141. X. Li, D.A. Brue, G.A. Parker, S. Chang, General laser interaction theory in atom-diatom systems for both adiabatic and non-adiabatic cases. J. Phys. Chem. A **110**, 5504–5512 (2006)
142. R.T. Pack, E.A. Butcher, G.A. Parker, Accurate 3D quantum probabilities and collision lifetimes of the $H+O_2$ combustion reaction. J. Chem. Phys. **102**, 5998–6012 (1995)
143. G.A. Parker, A. Laganà, S. Crocchianti, R.T. Pack, A detailed 3D quantum study of the Li + HF reaction. J. Chem. Phys. **102**, 1238–1250 (1995)
144. B.J. Archer, G.A. Parker, R.T. Pack, Positron-hydrogen atom S-wave coupled channel scattering at low energies. Phys. Rev. Lett. **41**, 1303–1310 (1990)
145. J.V. Lill, G.A. Parker, J.C. Light, The discrete variable-finite basis approach to quantum scattering. J. Chem. Phys. **85**, 900–910 (1986)
146. M. Keil, G.A. Parker, Empirical potential for the He + CO_2 interaction: multi-property fitting in the infnite-order sudden approximation. J. Chem. Phys. **82**, 1947–1966 (1985)
147. M. Keil, G.A. Parker, A. Kuppermann, An empirical anisotropic intermolecular potential for He + CO_2. Chem. Phys. Lett. **59**, 443–448 (1978)
148. G.A. Parker, R.T. Pack, Rotationally and vibrationally inelastic scattering in the rotational IOS approximation. Ultrasimple of total (differential, integral, and transport) cross sections for non-spherical molecules. J. Chem. Phys. **68**, 1585–1601 (1978)
149. A. Schawlow, T.W. Hnsch, G.W. Series, The spectrum of atomic hydrogen. Sci. Am. **240**, 94–111 (1979)
150. C. Manuali, A. Laganà, GRIF: a new collaborative framework for a web service approach to grid empowered calculations. Future Gener. Comput. Syst. **27**(3), 315–318 (2011)
151. https://www.fosteropenscience.eu/
152. H. Goldstein, *Classical Mechanics* (Addison Wesley, Tokyo, 1964)
153. D.M. Hirst, *Potential Energy Surfaces: Molecular Structures and dynamics* (Taylor & Francis Inc., London, 1985)