REFERENCES

[1] J.T. Hynes, J.P. Klinman, H.H. Limbach, R.L. Schowen, Hydrogen-transfer reactions: biological aspects I–II. WILEYVCH Verlag GmbH & Co. KGaA, Weinheim, 2007, pp 1–4.

[2] S.M. Chang, Y.J. Tzeng, S.Y. Wu, K.Y. Li, K.L, *Hsueh, Thin. Solid. Films*., 2005, 477: 38.

[3] R. Rey, K.B. Moller, J.T. Hynes, *J. Phys. Chem. A*, 2002, 106: 11993.

[4] L.G. Arnaut, S.J. Formosinho, *J. Photochem. Photobiol. A*, 1993, 199375: 1.

[5] S.J. Formosinho, L.G. Arnaut, *J Photochem Photobiol A*, 1993, 75: 21.

[6] J. Gebicki, T. Bally, *Acc. Chem. Res*., 1997, 30: 477.

[7] E. Freier, S. Wolf, K. Gerwert, *Proc. Natl. Acad. Sci. U.S.A.*., 2011, 108: 11435.

[8] A.H. Zewail, Pure. Appl. Chem., 2000, 200072: 2219.

[9] T.-I. Kim, H. J. Kang, G. Han, S. J. Chung, Y. Kim, *Chem. Commun. (Cambridge, U. K.)*, 2009, 5895.

[10] A. R. Morales, K. J. Schafer-Hales, C. O. Yanez, M. V. Bondar, O. V. Przhonska, A. I. Marcus, K. D. Belfield, *Chem. Phys. Chem.*, 2009, 10: 2073.

[11] F. S. Rodembusch, F. P. Leusin, L. F. da Costa Medina, A. Brandelli, V. Stefani, *Photochem. Photobiol. Sci.*, 2005, 4: 254.

[12] A. Kyrychenko, Y. Stepanenko, J. Waluk, *J. Phys. Chem.* A, 2000, 104: 9542.

[13] M. S. Gordon, *J. Phys. Chem.*, 1996, 100: 3974.

[14] A. Kyrychenko, J. Waluk, *J. Phys. Chem. A*, 2006, 110: 11958.

[15] J. Waluk, *Acc. Chem. Res.*, 2003, 36: 832.

[16] Y. Nosenko, M. Kunitski, R. P. Thummel, A. Kyrychenko, J. Herbich, J. Waluk, C. Riehn, B. Brutschy, *J. Am. Chem. Soc.*, 2006, 128: 10000.

[17] Y. Nosenko, A. Kyrychenko, R. P. Thummel, J. Waluk, B. Brutschy, J. Herbich, *Phys. Chem. Chem. Phys.*, 2007, 9: 3276.

[18] Y. Nosenko, M. Kunitski, C. Riehn, R. P. Thummel, A. Kyrychenko, J. Herbich, J. Waluk, B. Brutschy, *J. Phys. Chem. A*, 2008, 112: 1150.

[19] A. Fernández-Ramos, E. Martínez-Núñez, S. A. Vázquez, M. A. Ríos, C. M. Estévez, M. Merchán, and L. Serrano-Andrés, *J. Phys. Chem. A*, 2007, 111: 5907.

[20] M. Guglielmi, I. Tavernelli, U. Rothlisberger, *Phys. Chem. Chem. Phys.*, 2009, 11: 4549.

[21] S.-Y. Park, and D.-J. Jang, *J. Am. Chem. Soc.*, 2009, 132: 297.

[22] C. Tanner, C. Manca, S. Leutwyler, *Science (Washington, DC, U. S.)*, 2003, 302: 1736.

[23] C. Tanner, C. Manca, S. Leutwyler, *J. Chem. Phys.*, 2005, 122: 204326/204321.

[24] C. Tanner, M. Thut, A. Steinlin, C. Manca, S. Leutwyler, *J. Phys. Chem. A*, 2006, 110: 1758.

[25] J. Catalan, *J. Phys. Chem. A*, 2002, 107: 6738.

[26] J. Catalan, *Int. J. Quantum Chem.*, 2005, 102: 489.

[27] J. Catalan, V.J.C. del, M. Kasha, *Proc. Natl. Acad. Sci. U.S.A.*, 1999, 96: 8338.

[28] J. Catalan, P. Perez, V.J.C. del, P.J.L.G. de, M. Kasha, *Proc Natl Acad Sci U.S.A.*, 2004, 101: 419.

[29] C.-P. Chang, H. Wen-Chi, K. Meng-Shin, P.-T. Chou, J.H. Clements, *J. Phys. Chem.*, 1994, 98: 8801.

[30] Y. Chen, F. Gai, J.W. Petrich, *Chem. Phys. Lett.*, 1994, 222: 329.

[31] Y. Chen, R.L. Rich, F. Gai, J.W. Petrich, *J. Phys. Chem*., 1993, 97: 1770.

[32] P.T. Chou, M.L. Martinez, W.C. Cooper, S.T. Collins, D.P. McMorrow, M. Kasha, *J. Phys. Chem.*, 1992, 96: 5203.

[33] P.-T. Chou, C.-Y. Wei, C.-P. Chang, M.-S. Kuo, *J. Phys. Chem*., 1995, 99: 11994.

[34] P.-T. Chou, C.-Y. Wei, G.-R. Wu, W.-S. Chen, *J. Am. Chem. Soc*., 1999, 121: 12186.

[35] P.-T. Chou, W.-S. Yu, Y.-C. Chen, C.-Y. Wei, S.S. Martinez, *J. Am. Chem. Soc.*, 1998, 120: 12927.

[36] R. Daengngern, N. Kungwan, P. Wolschann, A.J.A. Aquino, H. Lischka, M. Barbatti, *J. Phys. Chem. A*, 2011, 115: 14129.

[37] R. Daengngern, K. Kerdpol, N. Kungwan, S. Hannongbua, M. Barbatti, *J. Photochem. Photobiol. A*, 2013, 266: 28.

[38] N. Kungwan, K. Kerdpol, R. Daengngern, S. Hannongbua, M. Barbatti, *Theor. Chem. Acc.*, 2014, 133: 1480.

[39] H. Fang, Y. Kim, *J. Phys. Chem. B*, 2011, 115: 15048.

[40] H. Fang, Y. Kim, *J. Phys. Chem. A*, 2011,115: 13743.

[41] H. Fang, Y. Kim, *J. Chem. Theory Comput*., 2011, 7: 642.

[42] D.E. Folmer, E.S. Wisniewski, S.M. Hurley, A.W. Castleman, Jr., *Proc. Natl. Acad. Sci. U. S. A.*, 1999, 96: 12980.

[43] D.E. Folmer, E.S. Wisniewski, J.R. Stairs, A.W. Castleman, *J. Phys. Chem. A*, 2000, 104: 10545.

[44] W.-T. Hsieh, C.-C. Hsieh, C.-H. Lai, Y.-M. Cheng, M.-L. Ho, K.K. Wang, G.-H. Lee, P.-T. Chou, *Chem. Phys. Chem*, 2008, 9: 293.

[45] Y. Kageura, K. Sakota, H. Sekiya, *J. Phys. Chem. A*, 2009, 113: 6880.

[46] K. Sakota, N. Inoue, Y. Komoto, H. Sekiya, *J. Phys. Chem. A*, 2007, 111: 4596.

[47] K. Sakota, C. Jouvet, C. Dedonder, M. Fujii, H. Sekiya, *J. Phys. Chem. A*, 2010, 114: 11161.

[48] K. Sakota, Y. Kageura, H. Sekiya, *J. Chem. Phys*., 2008, 129: 054303/054301.

[49] K. Sakota, Y. Komoto, M. Nakagaki, W. Ishikawa, H. Sekiya, *Chem. Phys. Lett*., 2007, 435: 1.

[50] K. Sakota, N. Komure, W. Ishikawa, H. Sekiya, *J. Phys. Chem.* A, 2009, 130: 224307/1.

[51] D. Kina, A. Nakayama, T. Noro, T. Taketsugu, M.S. Gordon, *J. Phys. Chem. A*, 2008, 112: 9675.

[52] Y. Koizumi, C. Jouvet, T. Norihiro, S.-i. Ishiuchi, C. Dedonder-Lardeux, M. Fujii, *J. Chem. Phys*., 2008, 129: 1043011/1.

[53] M. Klessinger, J. Michl, *Excited States and Photochemistry of Organic Molecules*. 1st ed. New York: VCH Publishers, 1995.

[54] B. Valeur, *Molecular Fluorescence Principles and Applications*. 1st ed. Paris: WILEY-VCH, 2002.

[55] G. C. Schatz, M. A. Ratner, *Quantum Mechanics in Chemistry*. New York: Dover Publications, Inc., 2001.

[56] D. C. Young, *Computational Chemistry: A Practical Guide for Applying Techniques to Real-World Problems*. New York: John Wiley & Sons, Inc., 2001.

[57] C. Hatting, *J. Chem. Phys*., 2003, 118: 7751.

[58] C. Hatting, *J. Adv. Quantum Chem*., 2005, 50: 37.

[59] M. Barbatti, R. Shepard, H. Lischka, *Computational and Methodological Elements for Nonadiabatic Trajectory Dynamics Simulations of Molecules*. Singapore: World Scientific, 2010.

[60] C.A. Taylor, M.A. El-Bayoumi, M. Kasha, *Proc. Natl. Acad. Sci. U.S.A*., 1969, 63: 253.

[61] H. Yokoyama, H. Watanabe, T. Omi, S. Ishiuchi, M. Fujii, *J. Phys. Chem. A*, 2001, 105: 9366.

[62] A. Nakajima, M. Hirano, R. Hasumi, K. Kaya, H. Watanabe, C.C. Carter, J.M. Williamson, T.A. Miller, *J. Phys. Chem. A*, 1997, 101: 392.

[63] A.S. Smirnov, D.S. English, R.L. Rich, J. Lane, L. Teyton, A.W. Schwabacher, S. Luo, R.W. Thornburg, J.W. Petrich, *J. Phys. Chem. B*, 1997, 101: 2758.

[64] M. Negrerie, F. Gai, S.M. Bellefeuille, J.W. Petrich, *J. Phys. Chem.*, 1991, 95: 8663.

[65] M. Negrerie, S.M. Bellefeuille, S. Whitham, J.W. Petrich, R.W. Thornburg, *J. Am. Chem. Soc*., 1990, 112: 7419.

[66] P.-T. Chau J., *Chin. Chem. Soc*., 2001, 48: 651.

[67] G.M. Chaban, M.S. Gordon, *J. Phys. Chem. A*, 1999, 103: 185.

[68] J.W. Young, D.W. Pratt, *J. Phys. Chem*., 2011, 135: 084301.

[69] M.P.T. Duong, Y. Kim, *J. Phys. Chem. A*, 2010, 114: 3403.

[70] Y. Huang, S. Arnold, M. Sulkes, *J. Phys. Chem*., 1996, 100: 4734.

[71] G.A. Pino, I. Alata, C. Dedonder, C. Jouvet, K. Sakota, H. Sekiya, *Phys. Chem. Chem. Phys*., 2011, 13: 6325.

[72] A. Fernandez-Ramos, Z. Smedarchina, W. Siebrand, M.Z. Zgierski, J. *Chem. Phys.*, 2001, 114: 7518.

[73] X. Yu, S. Yamazaki, T. Taketsugu, *J. Phys. Chem. A*, 2012, 116: 10566.

[74] A. Schafer, H. Horn, R. Ahlrichs, *J. Chem. Phys*., 1992, 97: 2571.

[75] R. Ahlrichs, M. Bar, M. Haser, H. Horn, C Kolmel, *Chem. Phys. Lett*., 1989, 162: 165.

[76] A. Schafer, C. Huber, R. Ahlrichs, *J. Chem. Phys*., 1994, 100: 5829.

[77] R. Casadesus, M. Moreno, J.M. Lluch, *Chem. Phys*., 2003, 290: 319.

[78] A.B. Trofimov, J. Schirmer, *J. Phys. B At. Mol. Opt. Phys*., 1995, 28: 2299.

[79] J. Schirmer, *Phys. Rev. A*, 1982, 26: 2395.

[80] N.O.C. Winter, N.K. Graf, S. Leutwyler, C. Hattig, *Phys. Chem. Chem. Phys*., 2013, 15: 6623.

[81] C. Hattig, F. Weigend, *J. Chem. Phys*., 2000, 113: 5154.

[82] M. Barbatti, M. Ruckenbauer, F. Plasser, J. Pittner, G. Granucci, M. Persico, H. Lischka, *WIREs Comput. Mol. Sci*., 2014, 4: 26.

[83] M. Barbatti, G. Granucci, M. Ruckenbauer, F. Plasser, R. Crespo-Otero, J. Pittner, M. Persico, H. Lischka, NEWTON-X: a package for Newtonian dynamics close to the crossing seam, 2013, www.newtonx.org.

[84] W.C. Swope, H.C. Andersen, P.H. Berens, K.R. Wilson, *J. Chem. Phys*., 1982, 76: 637.

[85] L. Verlet, *Phys. Rev*., 1967, 159: 98.

[86] N. Kungwan, R. Daengngern, T. Piansawan, S. Hannongbua, M. Barbatti, *Theor. Chem. Acc.*, 2013, 132: 1.

[87] N. Kungwan, F. Plasser, A.J.A. Aquino, M. Barbatti, P. Wolschann, H. Lischka, *Phys. Chem. Chem. Phys*.,2012, 14: 9016.

[88] M. Barbatti, A.J.A. Aquino, H. Lischka, C. Schriever, S. Lochbrunner, E. Riedle, *Phys. Chem. Chem. Phys*., 2009, 11: 1406.

[89] M.J.S. Dewar, *J. Am. Chem. Soc*., 1984, 106: 209.

[90] M. Lawrenz, R. Baron, J.A. McCammon, J. Chem. Theory. Comput., 2009, 5: 1106.

[91] D. Lu, G.A. Voth, *J. Am. Chem. Soc*., 1998, 120: 4006.

[92] H.S. Mei, M.E. Tuckerman, D.E. Sagnella, M.L. Klein, *J. Phys. Chem. B*, 1998, 102: 10446.

[93] R. Vuilleumier, D. Borgis, *J. Phys. Chem. B*, 1998, 102: 4261.

[94] P.T. Chou, S.L. Studer, M.L. Martinez, *Appl. Spectrosc*., 1991, 45: 513.

[95] S. Chang, E-Learning and Development of Adult Eduction, *Adult Education in China*, 2005, 38.

[96] S.M. Chang, K.L. Hsueh, B.K. Huang, J.H. Wu, C.C. Liao, K.C. Lin, *Surf. Coat. Technol*., 2006, 200: 3278.