

## Bibliography

- [1] A. Zewail and R. Bernstein, "Real-time laser femtochemistry: Viewing the transition from reagents to products," in *The Chemical Bond*, A. Zewail, ed., (Academic Press, Inc., Boston, 1992), pp. 223–279.
- [2] A. Zewail, *Femtochemistry – Ultrafast Dynamics of the Chemical Bond, Vols. I and II* (World Scientific, Singapore, 1994).
- [3] M. El-Sayed, I. Tanaka, and Y. Molin, *Ultrafast Processes in Chemistry and Photobiology – Chemistry for the 21st century* (IUPAC, Blackwell Scientific, Oxford, 1994).
- [4] D. Wiersma, *Femtosecond Reaction Dynamics* (Royal Academy of Arts and Sciences, North Holland, Amsterdam, 1994).
- [5] J. Manz and A. Castleman, Jr., "special issue on femtochemistry," *J. Phys. Chem.* **97**, 12423–12644 (1993).
- [6] *Femtosecond Chemistry*, J. Manz and L. Wöste, eds., (VCH, Weinheim, 1995), Vol. 1 and 2.
- [7] M. Chergui, *Femtochemistry – Ultrafast Chemical and Physical Processes in Molecular Systems* (World Scientific, Singapore, 1996).
- [8] *Ultrafast Phenomena XI*, T. Elsaesser, J. Fujimoto, D. A. Wiersma, and W. Zinth, eds., (Springer, Berlin, 1998).
- [9] A. H. Zewail, "Femtochemistry," *J. Phys. Chem. A* **104**, 5660–5694 (2000).
- [10] M. Shapiro and P. Brumer, "The equivalence of unimolecular decay product yields in pulsed and cw laser excitation," *J. Chem. Phys.* **84**, 540–541 (1986).
- [11] P. Brumer and M. Shapiro, "Control of unimolecular reactions using coherent light," *Chem. Phys. Lett.* **126**, 541–546 (1986).
- [12] P. Brumer and M. Shapiro, "Laser control of molecular processes," *Ann. Rev. Phys. Chem.* **43**, 257–282 (1992).
- [13] M. Shapiro, C. Zhidang, and P. Brumer, "Simultaneous control of selectivity and yield of molecular dissociation: pulsed incoherent interference control," *Chem. Phys.* **217**, 325–340 (1997).
- [14] B. Sheehy, B. Walker, and L. F. DiMauro, "Phase control in the two-color photodissociation of  $\text{HD}^+$ ," *Phys. Rev. Lett.* **74**, 4799–4802 (1995).
- [15] D. J. Tannor and S. A. Rice, "Control of selectivity of chemical reaction via control of wave packet evolution," *J. Chem. Phys.* **83**, 5013–5018 (1985).
- [16] R. I. Gordon and S. A. Rice, "Active control of the dynamics of atoms and molecules," *Am. Rev. Phys. Chem.* **48**, 601–641 (1987).

- [17] A. P. Peirce, M. A. Dahleh, and H. Rabiz, "Optimal control of quantum-mechanical systems: existence, numerical approximation, and applications," *Phys. Rev. A* **37**, 4950–4964 (1988).
- [18] R. I. Cukier, C. Denk, and M. Morillo, "Control of tunneling processes with an external field in a four-level system: an analytic approach," *Chem. Phys.* **217**, 179–199 (1997).
- [19] J. Cao and K. R. Wilson, "A simple physical picture for quantum control of wave packet localization," *J. Chem. Phys.* **107**, 1441–1450 (1997).
- [20] A. Rice and M. Zhao, *Optical control of molecular dynamics* (Wiley, New York, 2000).
- [21] Z. Li, R. Zadoyan, A. V. Apkarian, and C. C. Martens, "Femtosecond many-body dynamics of caging: Experiment and simulation of I<sub>2</sub> photodissociation-recombination in solid Ar," *J. Phys. Chem.* **99**, 7453–7465 (1995).
- [22] N. F. Scherer, D. M. Jonas, and G. R. Fleming, "Femtosecond wave packet and chemical reaction dynamics of iodine in solution: Tunable probe study of motion along the reaction coordinate," *J. Chem. Phys.* **99**, 153–168 (1993).
- [23] M. Sterling, R. Zadoyan, and V. A. Apkarian, "Interrogation and control of condensed phase chemical dynamics with linearly chirped pulses: I<sub>2</sub> in solid Kr," *J. Chem. Phys.* **104**, 6497–6506 (1996).
- [24] J. Xu, N. Schwentner, S. Hennig, and M. Chergui, "Ultrafast Intramolecular and Caging Dynamics of I<sub>2</sub> in CCl<sub>4</sub> from Resonance Raman Spectroscopy," *J. Raman Spectr.* **28**, 433–443 (1997).
- [25] R. Zadoyan, Z. Li, P. Ashjian, C. C. Martens, and V. A. Apkarian, "Femtosecond dynamics of coherent photodissociation-recombination of I<sub>2</sub> isolated in matrix Ar," *Chem. Phys. Lett.* **218**, 504–514 (1994).
- [26] R. Zadoyan, Z. Li, C. C. Martens, and V. A. Apkarian, "The breaking and remaking of a bond: Caging of I<sub>2</sub> in solid Kr," *J. Chem. Phys.* **101**, 6648–6657 (1994).
- [27] R. Zadoyan, M. Sterling, and V. A. Apkarian, "Dynamical spectroscopy of many-body interactions: Coherent vibrations and predissociation of I<sub>2</sub>(B) in solid Kr," *J. Chem. Soc., Faraday Trans.* **92**, 1821–1829 (1996).
- [28] R. Zadoyan, M. Sterling, M. Ovchinnikov, and V. A. Apkarian, "Predissociation Dynamics of I<sub>2</sub>(B) in Liquid CCl<sub>4</sub> Observed Through Femtosecond Pump-Probe Measurements: Electronic Caging Through Solvent Symmetry," *J. Chem. Phys.* **107**, 8446–8460 (1997).
- [29] R. Zadoyan, J. Almy, and V. A. Apkarian, "Lattice dynamics from the "eyes" of the chromophore - Real-time studies of I<sub>2</sub> isolated in rare gas matrices," *J. Chem. Soc., Faraday Trans.* **108**, 255–269 (1997).
- [30] A. V. Benderskii, R. Zadoyan, and V. A. Apkarian, "Caged Spin-Orbit Excited I\*(<sup>2</sup>P<sub>1/2</sub>) + I\*(<sup>2</sup>P<sub>1/2</sub>) Atom Pairs in Liquids and in Cryogenic Matrices: Spectroscopy and Dipolar Quenching," *J. Chem. Phys.* **107**, 8437–8445 (1997).
- [31] C. F. Bardeen, J. Che, K. R. Wilson, V. V. Yakovlev, V. A. Apkarian, C. C. Martens, R. Zadoyan, B. Kohler, and M. Messina, "Quantum control of I<sub>2</sub> in the gas phase and in condensed phase solid Kr matrix," *J. Chem. Phys.* **106**, 8486–8503 (1997).
- [32] M. Bargheer, K. Donovang, P. Dietrich, and N. Schwentner, "Extraction of potentials and dynamics from condensed-phase pump-probe spectra: Application to I<sub>2</sub> in Kr matrices," *J. Chem. Phys.* **111**, 8556–8564 (1999).

- 
- [33] I. Almy, K. Kizer, R. Zadoyan, and V. Apkarian, "Resonant Raman, Hot, and Cold Luminescence of Iodine in Rare Gas Matrixes," *J. Phys. Chem. A* **104**, 3508–3520 (2000).
- [34] T. Kobayashi and A. Shirakawa, "Tunable visible and near-infrared pulse generator in a 5 fs regime," *Appl. Phys. B* **70**, 239–246 (2000).
- [35] E. Riedle, M. Beutter, S. Lochbrunner, J. Piel, S. Schenkl, S. Sporlein, and W. Zinth, "Generation of 10 to 50 fs pulses tunable through all of the visible and the NIR," *Appl. Phys. B* **71**, 457–465 (2000).
- [36] V. A. Apkarian and N. Schwentner, "Molecular Photodynamics in Rare Gas Solids," *Chem. Rev.* **99**, 1481 – 1514 (1999).
- [37] M. Ovchinnikov and V. Apkarian, "Mixed-order semiclassical dynamics in coherent state representation: The connection between phonon sidebands and guest-host dynamics," *J. Chem. Phys.* **108**, 2277–2284 (1998).
- [38] R. B. Gerber, A. B. McCoy, and A. B. Garcia-Vela, "Photochemical reactions in weakly bound clusters," *Annu. Rev. Phys. Chem.* **45**, 275–314 (1994).
- [39] M. Gruebele, G. Roberts, M. Dantus, R. M. Bowman, and A. H. Zewail, "Femtosecond Temporal Spectroscopy and Direct Inversion to the Potential: Application to Iodine," *Chem. Phys. Lett.* **166**, 459–469 (1990).
- [40] C. Wan, M. Gupta, J. Baskin, Z. Kim, and A. Zewail, "Caging phenomena in reactions: Femtosecond observation of coherent, collisional confinement," *J. Chem. Phys.* **106**, 4353–4356 (1997).
- [41] Q. Liu, J.-K. Wang, and A. Zewail, "Femtosecond dynamics of dissociation and recombination in solvent cages," *Nature* **364**, 427–430 (1993).
- [42] C. Lienau and A. H. Zewail, "Femtochemistry at high pressures. Solvent effect in the gas-to-liquid transition region," *Chem. Phys. Lett.* **222**, 224–232 (1994).
- [43] C. Lienau, J. C. Williamson, and A. H. Zewail, "Femtochemistry at high pressures. The dynamics of an elementary reaction in the gas-liquid transition region," *Chem. Phys. Lett.* **213**, 289–296 (1993).
- [44] Q. Liu, C. Wan, and A. H. Zewail, "Femtosecond reaction dynamics in the gas-to-liquid transition region: Observation of a three-phase density dependence," *J. Chem. Phys.* **105**, 5294–5297 (1996).
- [45] R. Zadoyan, N. Schwentner, and V. A. Apkarian, "Wavepacket diagnosis with chirped probe pulses," *Chem. Phys.* **233**, 353 – 363 (1998).
- [46] M. Bargheer, M. Gühr, P. Dietrich, and N. Schwentner, "Femtosecond spectroscopy of fragment cage dynamics: I<sub>2</sub> in Kr," *Phys. Chem. Chem. Phys.* **4**, 75–81 (2002).
- [47] D. L. Huestis and N. E. Schlotter, "Diatomics-in-molecules potential surfaces for the triatomic rare gas halides: Rg<sub>2</sub>X," *J. Chem. Phys.* **69**, 3100–3107 (1978).
- [48] W. R. Wadt and P. Hay, "The low-lying electronic states of Ar<sub>2</sub>F," *Appl. Phys. Lett.* **30**, 573–575 (1977).
- [49] W. R. Wadt and P. J. Hay, "Electronic states of Ar<sub>2</sub>F and Kr<sub>2</sub>F," *J. Chem. Phys.* **68**, 3850–3886 (1978).

- [50] G. Hoffman and M. Colletto, "An ab initio study of some noble gas monohalides," *J. Chem. Phys.* **114**, 2219–2227 (2001).
- [51] T. H. Dunning, Jr. and P. J. Hay, "The covalent and ionic states of the rare gas monofluorides," *J. Chem. Phys.* **69**, 134–149 (1978).
- [52] *Excimer Lasers*, C. Rhodes, ed., (Springer-Verlag, Berlin Heidelberg, 1984).
- [53] H. Kunttu and V. Apkarian, "Photodissociation of F<sub>2</sub> in crystalline krypton: effect of molecule-lattice prealignment," *Chem. Phys. Lett.* **171**, 423–429 (1990).
- [54] H. Kunttu, J. Feld, R. Alimi, A. Becker, and V. Apkarian, "Charge transfer and radiative dissociation dynamics in fluorine-doped solid krypton and argon," *J. Chem. Phys.* **92**, 4856–4875 (1990).
- [55] R. Sauerbrey, Y. Zhu, F. K. Tittel, and W. L. Wilson, "Optical emission and kinetic reactions of four-atomic rare gas halide exciplex Ar<sub>3</sub>F," *J. Chem. Phys.* **85**, 1299–1302 (1986).
- [56] V. Aquilanti, D. Cappelletti, V. Lorent, E. Luzzatti, and F. Pirani, "Molecular beam studies of weak interactions of open-shell atoms: The ground and lowest excited states of rare-gas halides," *J. Phys. Chem.* **97**, 2063–2071 (1993).
- [57] V. Aquilanti, E. Luyyatti, F. Pirani, and G. G. Volpi, "Molecular beam studies of weak interactions for open-shell systems: The ground and lowest excited states of ArF, KrF and XeF," *J. Chem. Phys.* **89**, 6165–6175 (1988).
- [58] M. Ovchinnikov and V. A. Apkarian, "Quantum interference in resonant Raman spectra of I<sub>2</sub> in condensed media," *J. Chem. Phys.* **106**, 5775–5778 (1997).
- [59] A. A. Buchachenko and N. F. Stepanov, "Ar-I<sub>2</sub> interactions: The models based on the diatomics-in-molecule approach," *J. Chem. Phys.* **104**, 9913–9925 (1996).
- [60] M. Ben-Nun, R. D. Levine, and G. R. Fleming, "Solvent-induced nonadiabatic transitions in iodine: An ultrafast pump-probe computational study," *J. Chem. Phys.* **105**, 3035–3056 (1996).
- [61] M. Ben-Nun, R. D. Levine, D. M. Jonas, and G. R. Fleming, "Prompt solvent-induced electronic predissociation of femtosecond pumped iodine. A computational study," *Chem. Phys. Lett.* **245**, 629–638 (1995).
- [62] M. Ovchinnikov and V. A. Apkarian, "Condensed phase spectroscopy from mixed-order semiclassical molecular dynamics: Absorption, emission, and resonant Raman spectra of I<sub>2</sub> isolated in solid Kr," *J. Chem. Phys.* **105**, 10312–10331 (1996).
- [63] V. S. Batista and D. F. Coker, "Nonadiabatic molecular dynamics simulation of photodissociation and geminate recombination of I<sub>2</sub> liquid xenon," *J. Chem. Phys.* **105**, 4033–4054 (1996).
- [64] V. S. Batista and D. F. Coker, "Nonadiabatic molecular dynamics simulation of ultrafast pump-probe experiments on I<sub>2</sub> in solid rare gases," *J. Chem. Phys.* **106**, 6923–6941 (1997).
- [65] V. S. Batista and D. F. Coker, "Nonadiabatic molecular dynamics simulations of the photofragmentation and geminate recombination dynamics in size-selected I<sub>2</sub><sup>-</sup> Ar<sub>n</sub> cluster ions," *J. Chem. Phys.* **106**, 7102–7116 (1997), erratum: *J. Chem. Phys.* **110**, 6583–6584 (1999).
- [66] N. Yu, C. J. Margulis, and D. F. Coker, "Influence of solvation environment on excited state avoided crossings and photodissociation dynamics," *J. Phys. Chem. B* **105**, 6728–6737 (2001).
- [67] R. Alimi, R. B. Gerber, and V. A. Apkarian, "Dynamics of molecular reactions in solids: Photodissociation of F<sub>2</sub> in crystalline Ar," *J. Chem. Phys.* **92**, 3551–3558 (1990).

- 
- [68] K. S. Kizer and V. A. Apkarian, "Orbital alignment during cage-exit of open-shell photofragments: F in solid Ar and Kr," *J. Chem. Phys.* **103**, 4945–4952 (1995).
- [69] A. Krylov, R. Gerber, and V. Apkarian, "Adiabatic approximation and non-adiabatic effects for open-shell atoms in an inert solvent: F atoms in solid Kr," *Chem. Phys.* **189**, 261–272 (1994).
- [70] A. Krylov and R. Gerber, "Reorientation dynamics of electronic orbitals in condensed phases: Simulations of the  $F(^2P)$  atoms in solid Kr," *Chem. Phys. Lett.* **231**, 395 (1994).
- [71] M. Y. Niv, M. Bargheer, and R. B. Gerber, "Photodissociation and recombination of  $F_2$  molecule in  $Ar_5$  cluster: Nonadiabatic molecular dynamics simulations," *J. Chem. Phys.* **113**, 6660–6672 (2000).
- [72] R. B. Gerber, M. V. Korolkov, J. Manz, M. Y. Niv, and B. Schmidt, "A reflection principle for the control of molecular photodissociation in solids: model simulation for  $F_2$  in Ar," *Chem. Phys. Lett.* **327**, 76–84 (2000).
- [73] G. Chaban, R. Gerber, M. Korolkov, J. Manz, M. Niv, and B. Schmidt, "Photodissociation dynamics of molecular fluorine in an argon matrix induced by ultrashort laser pulses," *J. Phys. Chem. A* **105**, 2770–2782 (2001).
- [74] M. Jacox, "Comparison of the electronic energy levels of diatomic molecules in the gas-phase and in inert solid matrices," *J. Mol. Struct.* **157**, 43–59 (1987).
- [75] M. Chergui and N. Schwentner, "Cage Effect on the Photodissociation of Small Molecules in Van der Waals Clusters and Crystals," In *Trends in Chemical Physics*, D. J. Menon, ed., **2**, 89–113 (Trivandrum, India, 1992).
- [76] M. E. Jacox, "The vibrational energy levels of small transient molecules isolated in neon and argon matrices," *Chem. Phys.* **189**, 149–170 (1994).
- [77] V. Apkarian and V. Bondybey, "Special issue on: Photophysics of matrix isolated molecules," 1994.
- [78] V. E. Bondybey, A. M. Smith, and J. Agreiter, "New Developments in Matrix Isolation Spectroscopy," *Chem. Rev.* **96**, 2113–2134 (1996).
- [79] M. Macler and M. C. Heaven, "Spectroscopy and relaxation dynamics of metastable electronically excited states of iodine in rare gas matrices," *Chem. Phys.* **151**, 219–232 (1991).
- [80] J. Helbing and M. Chergui, "Solvation of ion-pair states in non-polar media:  $I_2$  in solid neon, argon and krypton," *J. Chem. Phys.* **115**, 6158–6172 (2001).
- [81] H. K. J. Feld and V. A. Apkarian, "Photodissociation of  $F_2$  and mobility of F atoms in crystalline argon," *J. Chem. Phys.* **93**, 1009 – 1020 (1990).
- [82] C. Bressler, *Spektroskopie und Photomobilität von Fluor in Edelgasmatrizen* (Wissenschaft und Technik Verlag, Berlin, 1995), ISBN 3-928943-24-3.
- [83] C. Bressler, W. G. Lawrence, and N. Schwentner, "Spectroscopy of  $F_2$  in Ne matrices," *J. Chem. Phys.* **105**, 1318–1329 (1996).
- [84] M. H. Hill and V. A. Apkarian, "Photodynamics of charge transfer and ion-pair states of  $Cl_2Xe$  complexes in liquid Ar," *J. Chem. Phys.* **105**, 4023–4032 (1996).
- [85] P. Beeken, E. A. Hanson, and G. J. Flynn, "Photochemical and photophysical dynamics of diatomic iodine isolated in a rare gas cage," *J. Chem. Phys.* **78**, 5892–5899 (1983).

- [86] R. Perutz, "Photochemical Reactions Involving Matrix-Isolated Atoms," *Chem. Rev.* **85**, 77–96 (1985).
- [87] R. Alimi, R. B. Gerber, and V. A. Apkarian, "Photodissociation dynamics of F<sub>2</sub> in solid Kr: Theory versus experiment," *Phys. Rev. Lett.* **66**, 1295–1297 (1991).
- [88] H. Kunttu, E. Sekreta, and V. A. Apkarian, "Photodissociation and charge transfer photodynamics in crystalline krypton doped with F<sub>2</sub> and Xe," *J. Chem. Phys.* **94**, 7819–7831 (1991).
- [89] C. Bressler and N. Schwentner, "Penetration depths of photomobilized F atoms from a sandwich experiment," *Phys. Rev. Lett.* **76**, 648–651 (1996).
- [90] M. Dickgießer and N. Schwentner, "Penetration depth of energetic F atoms from F<sub>2</sub> dissociation in layered rare gas samples," *J. Chem. Phys.* **113**, 8260–8265 (2000).
- [91] A. Holleman and E. Wiberg, *Lehrbuch der Anorganischen Chemie* (Walter de Gruyter, Berlin, New York, 1985).
- [92] F. Schreiner, J. Malm, and J. Hindman, "The preparation and nuclear magnetic resonance of krypton difluoride," *J. Am. Chem. Soc.* **87**, 25–28 (1965).
- [93] J. J. Turner and G. C. Pimentel, "Krypton fluoride: preparation by the matrix isolation technique," *Science* **140**, 974–975 (1963).
- [94] N. Bartlett and F. Sladky, "The chemistry of krypton, xenon and radon," University of California Radiation Laboratory Report 19658 (June 1970).
- [95] W. F. Howard, Jr. and L. Andrews, "Synthesis of noble-gas dihalides by laser photolysis of matrix-isolated halogens," *J. Am. Chem. Soc.* **96**, 7864–7868 (1974).
- [96] L. Khriachtchev, M. Petterson, N. Runeberg, J. Lundell, and M. Rasanen, "A stable argon compound," *Nature* **406**, 874–876 (2000).
- [97] R. Gerber, "private communication," 2001.
- [98] J.-C. Diels and W. Rudolph, *Ultrashort laser pulse phenomena* (Academic Press, New York, 1996).
- [99] J. Manz, "Molecular Wavepacket Dynamics: Theory For Experiments 1926-1996," In *Femtochemistry and Femtobiology*, V. Sundström, ed., pp. 1–222 (World Scientific, Singapore, 1997).
- [100] D. Tannor, *Introduction to Quantum Mechanics: A Time Dependent Perspective* (University Science Press, Sausalito, 2001).
- [101] P. Ehrenfest, "Bemerkung über die angenäherte Gültigkeit der klassischen Mechanik innerhalb der Quantenmechanik," *Z. Phys.* **45**, 455–457 (1927).
- [102] K. Thompson and N. Makri, "Rigorous forward-backward semiclassical formulation of many-body dynamics," *Rhys. Rev. E.* **59**, 4729–4732 (1999).
- [103] A. Donoso and C. Martens, "Quantum Tunneling Using Entangled Classical Trajectories," *Phys. Rev. Lett.* **87**, 223202 (2001).
- [104] J. Franck, "Elementary processes of photochemical reactions," *Trans. Faraday Soc.* **21**, 536–542 (1925).
- [105] L. Landau and E. Lifschitz, *Lehrbuch der theoretischen Physik* (Verlag Harri Deutsch, 1990), Vol. III, Quantenmechanik.

- 
- [106] C. Zener, "Non-adiabatic crossing of energy levels," Proc. R. Soc. **137**, 696–702 (1932).
- [107] A. Arthurs and A. Dalgarno, "The theory of scattering by a rigid rotator," Proc. R. Soc. A **256**, 540–551 (1960).
- [108] F. O. Ellison, "A Method of Diatomics in Molecule. I. General Theory and Application to H<sub>2</sub>O," J. Am. Chem. Soc. **69**, 3540–3544 (1963).
- [109] F. Naumkin, "The ArClF van der Waals complex as an example of how atoms inside a molecule interact with those outside," Chem. Phys. **213**, 33–43 (1996).
- [110] I. Last and T. George, "Semiempirical study of polyatomic rare gas halides: application to the Xe<sub>n</sub>Cl systems," J. Chem. Phys. **87**, 1183–1193 (1987).
- [111] I. Last and T. George, "Interaction of Xe<sup>+</sup> and Cl<sup>-</sup> ions and their formed molecules with a Xe solid," J. Chem. Phys. **86**, 3787–3794 (1987).
- [112] *The Diatomics-in-Molecules Method and the Chemical Bond*, Z. Maksic, ed., (Springer, New York, 1990).
- [113] J. Tully and R. Preston, "Trajectory surface hopping approach to nonadiabatic molecular collisions: The reaction of H<sup>+</sup> with D<sub>2</sub>," J. Chem. Phys. **55**, 562–572 (1971).
- [114] J. Tully, "Molecular dynamics with electronic transitions," J. Chem. Phys. **93**, 1061–1071 (1990).
- [115] M. Gühr, M. Bargheer, P. Dietrich, and N. Schwentner, "Predissociation and Vibrational Relaxation in the B state of I<sub>2</sub> in Kr Matrix," J. Phys. Chem. submitted (2002).
- [116] M. Gühr, "Schwingungsrelaxation und Prädissoziation von Jodmolekülen in Edelgasmatrizen," Diploma Thesis, Institut für Experimentalphysik, FU-Berlin, 2001.
- [117] B. Garraway and K.-A. Suominen, "Wave packet dynamics: New physics and chemistry in femto time," Rep. Prog. Phys. **58**, 365–419 (1995).
- [118] C. Cohen-Tannoudji, *Quantum Mechanics* (John Wiley and Sons, New York, 1977).
- [119] M. Klein and J. Venables, *Rare gas solids* (Academic Press, London, 1976).
- [120] M. Dickgiesser and N. Schwentner, "Optimization of Exciton-Induced Detection of Atoms at Interfaces," J. Phys. Chem. A **104**, 3743–3749 (2000).
- [121] A. B. Alekseyev, H. Liebermann, R. J. Buenker, and D. B. Kokh, "Relativistic configuration interaction study of the ClF molecule and its emission spectra from 0<sup>+</sup> ion-pair states," J. Chem. Phys. **112**, 2274–2284 (2000).
- [122] M. E. Fajardo, V. A. Apkarian, A. Moustakas, H. Krueger, and E. Weitz, "Absorption Spectra of Intermolecular Charge-Transfer Transitions between Xenon and Halogen Molecules (F<sub>2</sub>, Cl<sub>2</sub>, Br<sub>2</sub>) in liquid xenon," J. Phys. Chem. **92**, 357–360 (1988).
- [123] H. Kuzmany, *Festkörperspektroskopie* (Springer Verlag, Berlin, Heidelberg, 1990).
- [124] W. Fowler and W. Beall, *Physics of Color Centers* (Academic Press, New York, 1986), (eds.).
- [125] N. Schwentner, "Dynamics of localized excitations from energy and time resolved spectroscopy," Appl. Opt. **19**, 4104–4114 (1980).
- [126] K. Huang and A. Rhys, "A theory of light-absorption and non-radiative transitions in F-centers," Proc. Roy. Soc. London A **204**, 406–423 (1950).

- [127] D. Halliday, M. Potter, J. Mullins, and A. Brinkman, "Photoluminescence study of a bulk vapour grown CdTe crystal," *Journal of Crystal Growth* **220**, 30–38 (2000).
- [128] V. E. Bondybey and C. Fletcher, "Photophysics of Cl<sub>2</sub> in rare gas solids," *J. Chem. Phys.* **64**, 3615–3620 (1976).
- [129] H. H. Mohammed, A. M. Taleb, and J. Fournier, "Rare-gas matrix shift calculations of CO Cameron bands," *Chem. Phys.* **91**, 267–272 (1984).
- [130] N. Schwentner, C. Bressler, W. Lawrence, J. Xu, and M. Chergui, "Environmental effects on the energetics and photo-induced dynamics of molecular states," *Chem. Phys.* **189**, 205–216 (1994).
- [131] C. Bressler, W. Lawrence, and N. Schwentner, "Rydberg and charge transfer states of F atoms in neon matrices," *J. Chem. Phys.* **102**, 48–56 (1995).
- [132] B. Ault and L. Andrews, "Absorption and emission spectra of matrix-isolated *XeF*, *KrF*, *XeCl* and *XeBr*," *J. Chem. Phys.* **65**, 4192–4201 (1976).
- [133] V. A. Alekseev and D. W. Setser, "Optical-optical double-resonance spectroscopic study of four ion-pair states of ClF and identification of the ClF(*A*<sup>3</sup>Π<sub>1</sub>) valence state," *J. Chem. Phys.* **107**, 4771–4782 (1997).
- [134] P. Gürtler, H. Kunz, and J. LeCalvé, "VUV spectroscopy of the Cl<sub>2</sub> molecule trapped in pure neon, pure argon or mixed neon-argon matrices," *J. Chem. Phys.* **91**, 6020 – 6028 (1989).
- [135] E. U. Condon, "A theory of intensity distribution in band systems," *Phys. Rev.* **28**, 1182–1201 (1926).
- [136] M. Karavitis, R. Zadoyan, and V. Apkarian, "Time resolved coherent anti-Stokes Raman scattering of I<sub>2</sub> isolated in matrix argon: Vibrational dynamics on the ground electronic state," *J. Chem. Phys.* **114**, 4131–4140 (2001).
- [137] G. Herzberg, *Molecular Spectra and Molecular Structure. I. Spectra of Diatomic Molecules* (Van Nostrand Reinhold Co., New York, 1950).
- [138] L. Brus, "Electronic transition dipole moments and excited-state alignment in linear molecules, with application to diatomic rare gas halide," *J. Mol. Spectr.* **64**, 376–381 (1977).
- [139] H. Haken and H. Wolf, *Molekülphysik und Quantenchemie* (Springer, Berlin, 1998).
- [140] A. C. Albrecht, "Polarizations and Assignments of transitions: The method of photoselection," *J. Mol. Spectr.* **6**, 84–108 (1961).
- [141] J. Michl and E. Thulstrup, *Spectroscopy with polarized light* (VCH Publishers, New York, 1986).
- [142] D. S. Kliger, *Polarized Light in Optics and Spectroscopy* (Academic Press, Boston, 1990).
- [143] E. Schreiber, *Femtosecond real-time spectroscopy of small molecules and clusters*, *Springer Tr. Mod. Phys.* **143** (Springer Verlag, Berlin, 1998).
- [144] M. Bargheer, "Wellenpaketdynamik von Jodmolekülen in Krypton Matrizen," Diploma Thesis, Institut für Experimentalphysik, FU-Berlin, 1999.
- [145] V. A. Alekseev, D. W. Setser, and J. Tellinghuisen, "The D' → A' Transition in ClF," *J. Mol. Spectr.* **194**, 61 – 72 (1999).
- [146] V. A. Alekseev, D. W. Setser, and J. Tellinghuisen, "The A (<sup>3</sup>Π<sub>1</sub>) state of ClF," *J. Mol. Spectr.* **195**, 162 – 171 (1999).



- [147] V. A. Alekseev and D. W. Setser, "Electronic Spectroscopy and Structure of ClF," *Bulletin of the Korean Chemical Society* **21**, 9 – 22 (2000).
- [148] D. B. Kokh, V. A. Alekseev, and D. W. Setser, "Analysis of the bound-free emission spectra from the  $E(0^+)$  and  $f(0^+)$  ion-pair states of ClF to obtain potentials for the ion-pair and repulsive valence states," *J. Chem. Phys.* **109**, 1763–1771 (1998).
- [149] D. Pilipovich, H. H. Rogers, and R. D. Wilson, "Chlorine Trifluoride Oxide. II. Photochemical Synthesis," *Inorg. Chem.* **11**, 2192–2194 (1972).
- [150] G. P. Zhitneva, "Role of the reaction  $\text{ClF}_2 + \text{Cl} \rightarrow 2\text{ClF}$  in the photolysis of chlorine monofluoride," *Kinet. Katal.* pp. 690–694 (1986).
- [151] R. Steunenberg and R. Vogel, "The Absorption Spectrum of Fluorine," *J. Am. Chem. Soc.* **78**, 901–902 (1956).
- [152] A. L. G. Rees, "Electronic spectrum and dissociation energy of fluorine," *J. Chem. Phys.* **26**, 1567–1571 (1957).
- [153] J. B. Burkholder and E. J. Bair, "Potential energy parameters and shapes of the vibrational components of the 345 nm system of chlorine," *J. Phys. Chem.* **87**, 1859–1863 (1983).
- [154] H. Schmitz and H. Schumacher, "Das Absorptionsspektrum von  $\text{ClF}_3$ ," *Z. Naturforschung* **2a**, 363 (1947).
- [155] T. O. Nelson, D. W. Setser, and J. Qin, "Interpretation of the two-photon, laser-assisted reactions of xenon with  $\text{Cl}_2$ ,  $\text{F}_2$ , and ClF and krypton with  $\text{F}_2$ ," *J. Phys. Chem.* **97**, 2585–2595 (1993).
- [156] I. S. McDermid, "Potential-energy curves, Franck-Condon factors and laser excitation spectrum  $B^3\Pi(0^+) - X^1\Sigma^+$  system of chlorine monofluoride," *J. Chem. Soc., Faraday Trans. 2* **77**, 519–530 (1981).
- [157] R. Coombe, D. Pilipovich, and R. K. Horne, "Chemical Generation of Electronically Excited ClF ( $B^3\Pi_{0^+}$ ) and the  $B \rightarrow X$  Emission spectrum," *J. Phys. Chem* **82**, 2484 – 2489 (1978).
- [158] A. Alekseyev, "private communication."
- [159] A. H. Nielsen and E. A. Jones, "The analysis of the infrared spectrum of chlorine monofluoride," *J. Chem. Phys.* **19**, 1117 –1121 (1951).
- [160] J. A. Coxon, "Dissociation Energies of Diatomic Halogen Fluorides," *Chem. Phys. Lett.* **33**, 136 – 140 (1975).
- [161] G. Mamantov, E. J. Vasini, M. C. Moulton, D. G. Vickroy, and T. Maekawa, "Chlorine-Fluorine system at low temperatures: Characterization of the  $\text{ClF}_2$  radical," *J. Chem. Phys.* **54**, 3419–3421 (1971).
- [162] L. Andrews, F. Chi, and A. Arkell, "Matrix infrared spectrum and vibrational analysis of the FCIO intermediate," *J. Am. Chem. Soc.* **96**, 1997 (1974).
- [163] C. Naulin, J. Lambard, and R. Bougon, "Vibrational spectra of the chlorine monofluoride ClF in cryogenic solutions," *J. Chem. Phys.* **76**, 3371–3377 (1982).
- [164] M. Diegelmann, K. Hohla, and K. Kompa, "Interhalogen UV laser on the 285 nm band of ClF," *Opt. Commun.* **29**, 334–338 (1979).
- [165] M. Diegelmann, H. P. Grieneisen, K. Hohla, X.-Y. Hu, J. Krasinski, and K. L. Kompa, "New TEA-Lasers Based on  $D' \rightarrow A'$  Transitions in Halogen Monofluoride Compounds: ClF, BrF,

- IF,” *Appl. Phys.* **23**, 283 – 287 (1980).
- [166] M. Diegelmann, K. Hohla, F. Rebrost, and K. L. Kompa, “Diatomic interhalogen laser molecules: Fluorescence spectroscopy and reaction kinetics,” *J. Chem. Phys.* **76**, 1233 – 1246 (1982).
- [167] F. Alberti, K. Huber, and E. Looi, “The lowest Rydberg Complex of ClF:  $c^3\Pi$  and  $C^1\Pi$ ,” *J. Mol. Spectr.* **102**, 289–296 (1983).
- [168] K. Darvesh, R. Boyd, and S. Peyerimhoff, “Electronically excited states of chlorine monofluoride: a multi-reference configuration interaction study,” *Chem. Phys.* **121**, 361–369 (1988).
- [169] F.-M. Tao and W. Klemperer, “The van der Waals potential-energy surfaces and the structures of ArClF and ArCl<sub>2</sub>,” *J. Chem. Phys.* **97**, 440–451 (1992).
- [170] S. Harris, S. Novick, and W. Klemperer, “Intermolecular potential between an atom and a diatomic molecule: The structure of ArClF,” *J. Chem. Phys.* **61**, 193–197 (1974).
- [171] V. Sorokin and A. Chichinin, “The 248 nm photodissociation of ClF<sub>3</sub>: quantum yields for F and Cl atoms,” *Chem. Phys. Lett.* **280**, 141–144 (1997).
- [172] J. Qin, T. Nelson, and D. Setser, “Two-Photon Laser-Assisted Reaction between Xe and ClF,” *J. Phys. Chem.* **95**, 5374–5378 (1991).
- [173] E. S. Prochaska and L. Andrews, “Raman, infrared, and ultraviolet spectra of the chlorine difluoride free radical in solid nitrogen,” *Inorg. Chem.* **16**, 339–343 (1977).
- [174] A. Sannigrahi and S. Peyerimhoff, “Ab initio SCF and CI study of the electronic structure of chlorine difluoride cation and anion,” *Chem. Phys. Lett.* **119**, 119–122 (1985).
- [175] A. Sannigrahi and S. Peyerimhoff, “Ab initio SCF and CI study of the electronic structure and spectrum of the chlorine difluoride radical,” *Chem. Phys. Lett.* **114**, 6–9 (1985).
- [176] E. Prochaska, B. Ault, and L. Andrews, “Infrared, Raman and Ultraviolet Spectra of  $M^+ClF^-$  Species in Solid Argon,” *Inorg. Chem.* **16**, 2021–2023 (1977).
- [177] B. Ault, “A search for the HF<sub>2</sub> and HClF neutral free radicals isolated in argon matrices,” *J. Chem. Phys.* **68**, 4012–4016 (1978).
- [178] L. Andrews, F. Chi, and A. Arkell, “Matrix infrared spectrum and vibrational analysis of the FClO intermediate,” *J. Am. Chem. Soc.* **96**, 1997–2000 (1974).
- [179] P. Bagus, B. Liu, and H. S. III, “Electronic structure and properties of krypton difluoride,” *J. Am. Chem. Soc.* **94**, 6635–6641 (1972).
- [180] A. Boate, J. Morton, and K. Preston, “EPR spectrum of Kr<sub>2</sub>F,” *Chem. Phys. Lett.* **54**, 579–581 (1978).
- [181] E. Riedel, *Anorganische Chemie* (de Gruyter, Berlin, 1999).
- [182] I. S. McDermid and J. B. Laudenslager, “Perturbations in the B<sup>3</sup>π(0<sup>+</sup>) state of ClF: A new low-lying electronic state,” *Chem. Phys. Lett.* **79**, 370–374 (1981).
- [183] T. Wilhelm, J. Piel, and E. Riedle, “Sub-20-fs pulses tunable across the visible from a blue-pumped single-pass noncollinear parametric converter,” *Opt. Lett.* **22**, 1494–1496 (1997).
- [184] G. Cerullo, M. Nisoli, S. Stagira, and S. D. Silvestri, “Sub-8-fs pulses from an ultrabroadband optical parametric amplifier in the visible,” *Opt. Lett.* **23**, 1283–1285 (1998).

- 
- [185] A. Shirakawa, I. Sakane, and T. Kobayashi, "Pulse-front-matched optical parametric amplification for sub-10-fs pulse generation tunable in the visible and near infrared," *Opt. Lett.* **23**, 1292–1294 (1998).
- [186] R. Boyd, *Nonlinear Optics* (Academic Press, San Diego, 1992).
- [187] E. Riedle, private communication.
- [188] D. Kane and R. Trebino, "Characterization of arbitrary femtosecond pulses using frequency-resolved optical gating," *IEEE J. Quant. Electr.* **29**, 571–579 (1993).
- [189] R. Trebino and D. J. Kane, "Using phase retrieval to measure the intensity and phase of ultrashort pulses: frequency-resolved optical gating," *J. Opt. Soc. Am. A* **10**, 1101–1111 (1993).
- [190] N. Schmitt, "Phasen- und Amplitudenmessungen an ultrakurzen Lichtpulsen," Diploma Thesis, Institut für Experimentalphysik, FU-Berlin, 1996.
- [191] J. G. Caffrey, H. Kunz, and N. Schwentner, "Spectroscopy and photodissociation of chlorine monomers and clusters in Ar-matrices," *J. Chem. Phys.* **96**, 155 – 164 (1992).
- [192] T. Ishiwata, H. Takekawa, and K. Obi, "Measurements of the radiative lifetimes of the  $\text{Cl}_2$  ion-pair states by optical-optical double resonance," *Chem. Phys* **177**, 303 – 308 (1993).
- [193] C. Bressler, W. Lawrence, and N. Schwentner, "Spectroscopy of argon fluoride and krypton fluoride exciplexes in rare gas matrices," *J. Chem. Phys.* **105**, 10178–10188 (1996).
- [194] H. Kunz, "Photodissoziation von  $\text{Cl}_2$  in Edelgasmatrizen und spektroskopische Untersuchung der Dissoziationsfragmente," PhD Thesis, Freie Universität Berlin, 1991.
- [195] M. Bargheer, J. Pietzner, P. Dietrich, and N. Schwentner, "Ultrafast laser-control of ionic-bond formation:  $\text{ClF}$  in argon solids," *J. Chem. Phys.* **115**, 9827–9834 (2001).
- [196] M. Macler, M. Erickson, H.-S. Lin, and M. C. Heaven, "Electronic spectroscopy and fluorescence decay dynamics of matrix isolated  $\text{IBr}$ ," *J. Phys. Chem* **96**, 4301–4306 (1992).
- [197] V. E. Bondybey and L. E. Brus, "Rigid cage effect on  $\text{ICl}$  photodissociation and  $B\ 0^+$  fluorescence in rare gas matrices," *J. Chem. Phys.* **62**, 620–629 (1975).
- [198] J.-P. Nicolai and M. C. Heaven, "Laser excitation spectra for matrix isolated  $\text{IF}$ : observation of new low-lying electronic states," *J. Chem. Phys.* **87**, 3304 – 3312 (1987).
- [199] C. A. Wight, B. S. Ault, and L. Andrews, "Laser-induced fluorescence and resonance raman spectra of interhalogen diatomics isolated in inert matrices at 12K," *J. Mol. Spectr.* **56**, 239–250 (1975).
- [200] M. Bargheer, P. Dietrich, K. Donovang, and N. Schwentner, "Extraction of potentials and dynamics from condensed phase pump-probe spectra: Application to  $\text{I}_2$  in Kr matrices," *J. Chem. Phys.* **111**, 8556–8564 (1999).
- [201] G. Zerza, G. Slivinski, N. Schwentner, G. J. Hoffman, D. G. Imre, and V. A. Apkarian, "Spectroscopy of  $\text{XeF}$  in Ar and Ne Matrices," *J. Chem. Phys.* **99**, 8414–8423 (1993).
- [202] M. E. Fajardo and V. A. Apkarian, "Cooperative photoabsorption induced charge transfer reaction dynamics in rare gas solids. I. Photodynamics of localized xenon chloride exciplexes," *J. Chem. Phys.* **85**, 5660–5681 (1986).
- [203] M. Dickgießer and N. Schwentner, "Set-up combining synchrotron radiation-induced photochemistry with IR probing:  $(\text{HCl})_n$  in Kr matrix," *Nucl. Instr. Meth. B* **168**, 252–267 (2000).
- [204] V. S. Batista, C. Margulis, and D. Coker, private communication .

- [205] M. Bargheer, P. Dietrich, and N. Schwentner, "Spectroscopy and Photodissociation of ClF in Ar," *J. Chem. Phys.* **115**, 149–157 (2001).
- [206] K. P. Huber and G. Herzberg, *Molecular Spectra and Molecular Structure. IV. Constants of Diatomic Molecules* (Van Nostrand Reinhold, New York, 1979).
- [207] R. Rydberg, "Graphische Darstellung einiger bandenspektroskopischer Ergebnisse," *Z. Phys.* **73**, 376–385 (1931).
- [208] O. Klein, "Zur Berechnung von Potentialkurven für zweiatomige Moleküle mit Hilfe von Spektraltermen," *Z. Phys.* **76**, 226–235 (1932).
- [209] A. Rees, "The calculation of potential-energy curves from band-spectroscopic data," *Proc. Phys. Soc. London A* **59**, 998–1008 (1947).
- [210] L. D. Landau and E. M. Lifschitz, *Lehrbuch der theoretischen Physik* (Akademie-Verlag, Berlin, 1979), Vol. I: Mechanik, Chap. 12.
- [211] H. Dietz, G. Knopp, A. Materny, and V. Engel, "The perturbation of coherent wave-packet dynamics by atom-molecule collisions: the NaI + Ar system," *Chem. Phys. Lett.* **275**, 519–526 (1997).
- [212] A. Heidenreich and J. Jortner, "Pump-Probe spectroscopy of ultrafast structural relaxation of electronically excited rare gas heteroclusters," *J. Electr. Spectr.* **106**, 187–197 (2000).
- [213] A. Goldberg and J. Jortner, "Structural Relaxation Dynamics of Electronically Excited XeAr<sub>N</sub> Clusters," *J. Chem. Phys.* **107**, 8994–9017 (1997).
- [214] C. Jeannin, M. Portella-Oberli, S. Jimenez, F. Vigliotti, B. Lang, and M. Chergui, "Femtosecond dynamics of electronic 'bubbles' in solid argon: viewing the inertial response and the bath coherences," *Chem. Phys. Lett.* **316**, 51–59 (2000).
- [215] S. Jimenez, M. Chergui, G. Rojas-Lorenzo, and J. Rubayo-Soneira, "The medium response to an impulsive redistribution of charge in solid argon: Molecular dynamics simulations and normal mode analysis," *J. Chem. Phys.* **114**, 5264–5272 (2001).
- [216] J. Baskin, M. Gupta, M. Chachisvilis, and A. Zewail, "Femtosecond dynamics of microscopic friction: nature of coherent versus diffusive motion from gas to liquid density," *Chem. Phys. Lett.* **275**, 437–444 (1997).
- [217] J. Baskin, M. Chachisvilis, M. Gupta, and A. Zewail, "Femtosecond dynamics of solvation: Microscopic friction and coherent motion in dense fluids," *J. Phys. Chem. A* **102**, 4158–4171 (1998).
- [218] I. Benjamin and K. Wilson, "Proposed experimental probes of chemical reaction molecular dynamics in solution: ICN photodissociation," *J. Chem. Phys.* **90**, 4176–97 (1989).
- [219] M. Levenson and S. Kano, *Introduction to Nonlinear Laser Spectroscopy* (Academic Press, Boston, 1988).
- [220] V. Bondybey and L. Brus, "Rigid cage photodissociation dynamics: A double minimum problem for ICl in Ne and Ar lattices," *J. Chem. Phys.* **64**, 3724–3731 (1976).
- [221] A. I. Krylov and R. B. Gerber, "Photodissociation dynamics of HCl in solid Ar: Cage exit, nonadiabatic transitions, and recombination," *J. Chem. Phys.* **106**, 6574–6587 (1997).
- [222] M. Y. Niv, A. I. Krylov, and R. B. Gerber, "Photodissociation, electronic relaxation and recombination of HCl in Ar<sub>n</sub>(HCl) clusters - Non-adiabatic molecular dynamics simulations,"

- 
- Faraday Discuss. **108**, 243–254 (1997).
- [223] T. Brixner, N. Damrauer, P. Niklaus, and G. Gerber, “Photosensitive adaptive femtosecond quantum control in the liquid phase,” *Nature* **414**, 57–60 (2001).
- [224] B. Friedrich and D. Herschbach, “Alignment and trapping of molecules in intense laser fields,” *Phys. Rev. Lett.* **74**, 4623–4626 (1995).
- [225] J. Larsen, I. Wendt-Larsen, and H. Stapelfeldt, “Controlling the Branching Ratio of Photodissociation Using Aligned Molecules,” *Phys. Rev. Lett.* **83**, 1123–1126 (1999).
- [226] J. Larsen, K. Hald, N. Bjerre, and H. Stapelfeldt, “Three dimensional Alignment of Molecules Using Elliptically Polarized Laser Fields,” *Phys. Rev. Lett.* **85**, 2470–2473 (2000).