Further Reading

[1] T. S. Kuhn, *The Structure of Scientific Revolutions*, University of Chicago Press, **1962**.

Kuhn's treatise on scientific revolutions is a classic, and a must-read for every scientist. See also the citations given in the text for more up-to-date views on Kuhn's work. Some scientific revolutions have not occurred quite as suddenly as Kuhn's notion of the paradigm shift seems to suggest.

[2] J. R. Gribbin, *In Search of Schrödinger's Cat: Quantum Physics and Reality*, Bantam Books, **1984**.

Based on the recommendation of a fellow student, I read this book right around the time when I took my first QM class as a college student, and I enjoyed it tremendously. Gribbin's book covers the endlessly fascinating history of QM and the people who discovered it, its strange implications, and its impact on modern life.

[3] J. P. McEvoy and O. Zarate, *Introducing Quantum Theory: A Graphic Guide to Science's Most Puzzling Discovery*, multiple publishers, **2003**. Originally published in the UK and Australia under the title *Quantum Theory for Beginners*, **1996**.

This is an easily readable and highly entertaining account of the history of QM and its strange predictions in the form of a graphic novel.

[4] R. A. Wilson, *Quantum Psychology: How Brain Software Programs You and Your World*, New Falcon Press, **1990**. Second edition published by Hilaritas Press, **2016**.

The late Robert Anton Wilson is one of my favorite authors. In this book, Wilson tries to apply some of the lessons learned from QM to human psychology. For example, instead of saying that something, or someone, *is* a certain way, it is usually better to state what one has observed about said person or object.

[5] R. G. Parr and W. Yang, *Density functional theory of atoms and molecules*, Oxford University Press, **1989**.

This book provides an introduction to, and an in-depth treatment of, DFT and KS theory as applied to atomic and molecular electronic structures. Important developments have taken place in the DFT field since this book was published, some of which are covered in the DFT and time-dependent DFT references given herein. A recommended on-line resource is Kieron Burke's 'ABC of DFT', available at https://dft.uci.edu/doc/g1.pdf (accessed January 2020).

[6] R. Hoffmann, *Solids and Surfaces: A Chemist's View of Bonding in Extended Structure*, Wiley-VCH, **1988**.

This is a short and very insightful book that introduces band-structure concepts to chemists and bridges the language gap between chemistry and condensed matter physics. Hoffmann illustrates beautifully how the chemical concepts of bonding can be applied to periodic systems in one, two, and three dimensions.

[7] N. W. Ashcroft and N. D. Mermin, *Solid State Physics*, Thomson Learning Inc., **1976**.

Ashcroft and Mermin's is a 'classic' text on condensed matter physics. Because of its publication date, it does not include many important developments that have taken place since—for example, in high-temperature superconductivity. Nonetheless, the book is an excellent resource if you want to learn more about solid state electronic structure. Among the more recently published condensed matter physics textbooks are the following two references.

[8] R. M. Martin, *Electronic Structure: Basic Theory and Practical Methods*, Cambridge University Press, **2004**.

This book presents electronic structure methods from the band structure/condensed matter viewpoint. Among other topics, the text covers density functional methods and response theory for solids.

[9] M. L. Cohen and S. G. Louie, *Fundamentals of Condensed Matter Physics*, Cambridge University Press, **2016**.

This is another recommended resource if you want to learn more about condensed matter theory.

[10] G. B. Arfken, H. J. Weber, and F. E. Harris, *Mathematical Methods for Physicists: A Comprehensive Guide*, 7th edition, Academic Press, **2012**.

This comprehensive textbook covers a wide range of mathematical methods used widely in science and engineering. The title may well read '. . . *for Physicists and Physical Chemists*'. Fourier transforms, special functions, the particle in a sphere, and much more are covered.

[11] F. W. Byron and R. W. Fuller, *The Mathematics of Classical and Quantum Physics*, Addison-Wesley, **1969**. Corrected Dover republication, **1992**.

This is another 'Mathematics for . . .' text that I consulted frequently while working on this book. The introduction of response functions and the derivation of the Kramers-Kronig transformations presented in Chapter 23 closely follows the presentation of Byron and Fuller.

[12] I. N. Levine, *Quantum Chemistry*, 7th edition, Pearson, **2014**.

As a student, I learned a lot of quantum chemistry from previous editions of Levine's book. It is referenced in several places in the text, where I took some shortcuts, regarding further details and derivations.

[13] A. Szabo and N. S. Ostlund, *Modern Quantum Chemistry: Introduction to Advanced Electronic Structure Theory*, Dover, **1996**.

Szabo and Ostlund's book is highly recommended reading if you want to explore additional technical aspects of Hartree-Fock (HF) theory, or if you want to learn more about electron correlation methods (post-HF), the calculation of molecular integrals with Gaussian-type basis functions, and other topics such as diagrammatic perturbation theory. The reference is to a revised Dover reprint of the original 1982 publication. For a more up-to-date account on electronic structure methods, see [14].

[14] T. Helgaker, P. Jørgensen, and J. Olsen, *Molecular Electronic-Structure Theory*, Wiley, **2000**.

A comprehensive, modern, and technical treatise of the title subject. If you want to become an expert in molecular electronic structure, this is likely where you will either start reading or eventually get to.

[15] R. McWeeny, *Methods of Molecular Quantum Mechanics*, 2nd edition, Academic Press, **1992**.

This is an older, but still relevant, book on electronic structure and response methods, recommended for advanced readers.

[16] D. B. Cook, *Handbook of Computational Quantum Chemistry*, Oxford University Press, **1998**. Dover republication, **2005**.

This book is a useful resource if you want to learn how to program quantum chemistry methods. It covers a wide range of theoretical methods and includes pseudocode to show how the equations can be translated to a high-level programming language.

[17] L. Piela, *Ideas of Quantum Chemistry*, 2nd edition, Elsevier, **2014**.

This is a very ambitious textbook, covering a very wide range of quantum chemistry concepts and their applications. Piela illustrates the many branches of molecular electronic structure theory with a tree, with the QM postulates at the bottom of the trunk.

[18] L. D. Barron, *Molecular Light Scattering and Optical Activity*, 2nd edition, Cambridge University Press, edition, **2004**.

Barron provides a comprehensive treatment of the interactions between molecules and electromagnetic fields, with an emphasis on electronic and vibrational optical activity, both natural and induced. Molecule–field interactions are also explored in detail in P. W. Atkins and R. S. Friedman, *Molecular Quantum Mechanics*, 5th edition, Oxford University Press, **2011**; and G. C. Schatz and M. A. Ratner, *Quantum Mechanics in Chemistry*, Prentice Hall, **1993**. Dover republication, **2002**.

[19] P. Norman, K. Ruud, and T. Saue, *Principles and Practices of Molecular Properties: Theory, Modeling, and Simulations*, Wiley, **2018**.

This is a thorough and comprehensive treatment of static and dynamic response theory for molecules. Unlike Chapter 23, where we formulated linear and nonlinear response functions for exact states, with few exceptions, Norman, Ruud, and Saue show in detail also how response functions and their residues can be calculated within approximate variational and nonvariational electronic structure methods. An exhaustive account of static response methods applied within approximate electronic structure wavefunction methods, with many references to the original literature, can also be found in Y. Yamaguchi, Y. Osamura, J. D. Goddard, and H. F. Schaefer III, *A New Dimension to Quantum Chemistry: Analytic Derivative Methods in Ab Initio Molecular Electronic Structure Theory*, Oxford University Press, **1994**.

[20] K. G. Dyall and K. Fægri, Jr., *Relativistic Quantum Chemistry*, Oxford University Press, **2007**.

Dyall and Fægri's is among the more recent textbooks dedicated to relativistic QT as applied to atomic and molecular electronic structure.

[21] M. Reiher and A. Wolf, *Relativistic Quantum Chemistry: The Fundamental Theory of Molecular Science*, 2nd edition, Wiley-VCH, **2015**.

Reiher and Wolf's text on relativistic QT provides a comprehensive (broad and in-depth) description of the topic, with a large number of references to the original literature.

[22] R. E. Moss, *Advanced Molecular Quantum Mechanics*, Chapman and Hall, **1973**.

This is a textbook on relativistic molecular QM that I found very useful during my college and postdoc years. A soft cover reprint of the original first edition is currently available from Springer.

[23] H. A. Bethe and E. E. Salpeter, *Quantum Mechanics of One and Two Electron Atoms*, Academic Press and Springer, **1957**. Republication by Dover Publications, **2008**.

This is among the books in my collection with the highest equation density. As the title indicates, Bethe and Salpeter treat the theory of one- and two-electron atoms very thoroughly.

[24] D. C. Lay, S. R. Lay, and J. J. McDonald, *Linear Algebra and its Applications*, 5th edition, Pearson, **2016**.

An older edition of this book is one of the references I consulted while writing Appendix B.

[25] F. A. Cotton, *Chemical Applications of Group Theory*, 3rd edition, Wiley, **1990**.

Cotton's textbook on molecular symmetry and group theory is popular among chemists. As with books on other subjects in this list, there is a lot of choice among different authors.

[26] P. R. Bunker and P. Jensen, *Fundamentals of Molecular Symmetry*, Institute of Physics Publishing, **2005**.

This text presents symmetry concepts in the context of small-molecule spectroscopy.

[27] M. Hamermesh, *Group Theory and Its Application to Physical Problems*, Addison-Wesley, **1962**. Dover republication, **1989**.

This Dover reprint of Hamermesh's text is among the many available books that treat group theory and group representation theory in depth, with a focus on applications in physics.

[28] S. L. Altmann and P. Herzig, *Point-Group Theory Tables*, 2nd edition, Clarendon Press, **2011**.

This book presents working equations and complete information on the structures and properties of symmetry point groups, along with character and multiplication tables for 75 point groups, the associated double groups, descent-of-symmetry tables, and much more. A highly recommended resource. At the time of writing, the book is available as a free download from the University of Vienna (https://phaidra.univie.ac.at/view/o:104731).