

Contents

1	Quantum Chemistry	1
1.1	History of Quantum Chemistry	1
1.2	History of Theoretical Chemistry Prior to the Advent of Quantum Chemistry	6
1.3	Analytical Mechanics Underlying the Schrödinger Equation	11
1.4	Schrödinger Equation	15
1.5	Interpretation of the Wavefunction	17
1.6	Molecular Translational Motion	19
1.7	Molecular Vibrational Motion	22
1.8	Molecular Rotational Motion	25
1.9	Electronic Motion in the Hydrogen Atom	29
	References	31
2	Hartree–Fock Method	35
2.1	Hartree Method	35
2.2	Molecular Orbital Theory	38
2.3	Slater Determinant	42
2.4	Hartree–Fock Method	43
2.5	Roothaan Method	47
2.6	Basis Function	50
2.7	Coulomb and Exchange Integral Calculations	53
2.8	Unrestricted Hartree–Fock Method	56
2.9	Electronic States of Atoms	59
	References	63
3	Electron Correlation	65
3.1	Electron Correlation	65
3.2	Dynamical and Nondynamical Correlations	67
3.3	Configuration Interaction	70
3.4	Brillouin Theorem	73
3.5	Advanced Correlation Theories	75
	References	77

4	Kohn–Sham Method	79
4.1	Thomas–Fermi Method	79
4.2	Hohenberg–Kohn Theorem	80
4.3	Kohn–Sham Method	83
4.4	Generalized Kohn–Sham Method	85
4.5	Constrained Search Method for Constructing Kohn–Sham Potentials	87
4.6	Time-Dependent Kohn–Sham Method	90
4.7	Coupled Perturbed Kohn–Sham Method	94
	References	99
5	Exchange–Correlation Functionals	101
5.1	Classification of Exchange–Correlation Functionals	101
5.2	LDA and GGA Exchange Functionals	103
5.3	LDA and GGA Correlation Functionals	107
5.4	Meta-GGA Functionals	114
5.5	Hybrid Functionals	118
5.6	Semiempirical Functionals	120
	References	123
6	Corrections for Functionals	125
6.1	Long-Range Correction	125
6.2	Self-interaction Correction	130
6.3	van der Waals Correction	134
6.4	Relativistic Corrections	144
6.5	Vector Potential Correction and Current Density	152
	References	158
7	Orbital Energy	161
7.1	Koopmans Theorem	161
7.2	Janak’s Theorem	163
7.3	The Indispensability of Producing Accurate Orbital Energies	166
7.4	Electron Correlation Effects on Orbital Energies	169
7.5	Optimized Effective Potential Method	170
7.6	Highly Correlated Correlation Potentials	172
7.7	Constrained Search for Exact Potentials	175
7.8	Corrections for Orbital Energy Gaps in Solids	176
7.9	Orbital Energy Reproduction by Long-Range Corrected DFT	180
	References	187
8	Appendix: Fundamental Conditions	189
	References	195
	Index	197

Density Functional Theory in Quantum Chemistry

Tsuneda, T.

2014, X, 200 p. 25 illus., Hardcover

ISBN: 978-4-431-54824-9