

CONTENTS

VOLUME 2: APPLICATIONS

NOTE ON UNITS

xii

6 THERMODYNAMIC PROPERTIES OF PURE FLUIDS	627	8.6 Local mean field density functional theory	956
6.1 The energy equation	628	8.7 Non-local density functional theory	970
6.2 The pressure equation	630	8.8 Integral equation theory	978
6.3 The compressibility equation	631	8.9 Experimental and simulation studies of surface orientation	990
6.4 The free energy equation	632	8.10 Conclusions	1028
6.5 The test particle expressions for thermodynamic properties	633	Appendix 8A Functionals	1028
6.6 Thermodynamic properties in terms of spherical harmonic expansion coefficients	639	Appendix 8B Derivatives with respect to surface area	1038
6.7 Thermodynamic properties in terms of the site-site correlation functions	642	Appendix 8C Derivation of the angular gradient equations (8.25) and (8.26)	1041
6.8 A rigorous inequality for the free energy	652	Appendix 8D The Maxwell equations for macroscopic electrostatics	1042
6.9 Quantum corrections	653	Appendix 8E Simplified derivation of quadrupolar surface potential term	1044
6.10 Virial coefficients	658	References and notes	1047
6.11 Perturbation theory results	667	9 STRUCTURE FACTOR	1071
6.12 Hard nonspherical molecules: scaled particle and related theories	676	9.1 Scattering theory	1072
6.13 Associating fluids	693	9.2 Structure factor for a molecular fluid	1084
6.14 Nano-scale systems	733	9.3 Perturbation theory	1088
6.15 Conclusion	734	9.4 Integral equations	1095
Appendix 6A Geometry of convex bodies	735	9.5 Computer simulations and comparison with experiment	1102
References and notes	746	Appendix 9A Pressure derivative of $S(k)$	1130
7 THERMODYNAMIC PROPERTIES OF MIXTURES	761	Appendix 9B Body-fixed spherical harmonic coefficients of molecular form factors	1131
7.1 Qualitative behaviour	762	References and notes	1132
7.2 Kirkwood-Buff theory (KBT)	785	10 DIELECTRIC PROPERTIES	1143
7.3 The ideal mixture	801	10.1 Introduction	1143
7.4 Nonideal mixtures: the activity coefficient	804	10.2 Microscopic and macroscopic theories	1144
7.5 Dilute mixtures	807	10.3 Rigid polar fluids	1145
7.6 Fugacity and the Henry constant	810	10.4 Polarizable fluids	1150
7.7 Theory of simple mixtures: spherical molecules	811	10.5 Perturbation theory	1154
7.8 Perturbation theory: nonspherical molecules	831	10.6 Dielectric virial expansions	1158
7.9 Associating mixtures	851	10.7 Computer simulation	1173
7.10 Conclusions	871	10.8 Anisotropic fluids	1187
Appendix 7A Derivation of Eq. (7.51)	873	Appendix 10A Dielectric response in nonuniform fields	1198
Appendix 7B Application of Kirkwood-Buff Theory: supercritical fluid extraction	874	Appendix 10B The Clausius-Mossotti equation	1206
References and notes	877	Appendix 10C Perturbation theory for the angular correlation parameters G_l	1209
8 SURFACE PROPERTIES	887	Appendix 10D Ewald sums for ionic and dipolar systems	1211
8.1 Distribution functions and molecular alignment	888	Appendix 10E Integral equations and the dielectric constant	1216
8.2 Surface tension	905	References and notes	1220
8.3 Pressure tensor	928	11 SPECTROSCOPIC PROPERTIES	1230
8.4 Density functional theory	942	11.1 Infrared spectra	1231
8.5 Perturbation theory	946	11.2 Raman spectra	1270
		11.3 Neutron scattering	1314
		Appendix 11A Kramers-Kronig relations	1364
		References and notes	1369
		INDEX	1381