

Contents

1. Introduction	1
2. The Scope of Theoretical Methods	7
2.1 Electronic Structure Calculations	9
2.1.1 Perfect Crystals	15
2.1.2 Defective Crystals	18
2.2 Potential Simulations	33
2.2.1 Potential Forms and Applications	33
2.2.2 Derivation of Effective Crystal Potentials	40
3. Barium Titanate	49
3.1 Ferroelectricity of ABO_3 Perovskites	51
3.2 Defect Chemical Properties of Barium Titanate	54
3.3 Electronic Structure Calculations	58
3.3.1 Embedded Cluster Calculations for Transition Metal Ions in BaTiO_3	61
3.3.2 Simulation of Trapped Holes	77
3.3.3 Simulation of Electron-Type Bipolarons	97
3.3.4 Embedded Cluster Calculations of Oxygen Vacancies in BaTiO_3	98
4. Potassium Niobate and Potassium Tantalate	105
4.1 Shell Model Simulations in KNbO_3 and KTaO_3	106
4.1.1 Shell Model Parameters and Perfect Lattice Simulations	106
4.1.2 Defect Chemistry of KTaO_3 and KNbO_3	114
4.2 Polarizing Defect Centres	119
4.2.1 Dipole Formation Due to Off-Centre Displacements of Defects	122
4.2.2 Dipole Centres Due to Defect Aggregation	132
5. Lithium Niobate	147
5.1 Electronic Structure Calculations	147
5.2 Shell Model Simulations of Defect Chemical Properties	150

VIII Contents

5.2.1 Intrinsic Defect Structure.....	150
5.2.2 Incorporation of Impurities	154
6. Strontium Barium Niobate	161
7. Yttrium Iron Garnet	165
7.1 Potential Models	165
7.2 Chemical Stability of YIG	168
7.3 Intrinsic Defect Structures	170
7.4 Intrinsic Electronic Properties.....	173
7.5 Impurities	179
7.5.1 Incorporation of Trivalent Impurities.....	181
7.5.2 Incorporation of Divalent and Tetravalent Impurities ..	184
8. Summary and Conclusions.....	191
References	193
Index	203

