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2.2.5 The Na2SbF5 Crystal2.2.6 KB5O8 4H2O or K[B5O6(OH)4] 2H2O (KB5) Crystal; 2.2.7 The NaNO2 Crystal; 2.3 The Relationship between the Anionic Group and the Absorption Edge of Inorganic Crystals on the UV Side; 2.3.1 The Model and Approximation; 2.3.2 Absorption Edge Calculations for the Isolated Anionic Group Type; 2.3.2.1 Electronic Structure of -BaB2O4 (BBO); 2.3.2.2 Electronic Structure of LiB3O5 (LBO); 2.3.2.3 Electronic Structure of KBe2BO3F2 (KBBF); 2.3.2.4 Electronic Structure of KB5O8 4H2O; 2.3.2.5 Electronic Structure of KH2PO4 (KDP); 2.3.2.6 Electronic Structure of Na2SbF5
2.3.2.7 Electronic Structure of Iodate Crystals and NaNO2 Crystal2.3.3 Summary; 2.4 Ab initio Calculations on the Linear and Nonlinear Optical Properties of Borate and Other Crystals; 2.4.1 Computational Methods; 2.4.2 Calculations and Analysis for Borate Crystals; 2.4.2.1 BBO and LBO Family Crystals; 2.4.2.2 KBBF, BaAlBO3F2 (BABF) and Sr2Be2B2O7 (SBBO) Family Crystals; 2.4.2.3 BIBO Crystal; 2.4.3 Calculations and Analysis for Other NLO Crystals; 2.4.3.1 NaNO2; 2.4.3.2 Na2SbF5; 2.4.3.3 KH2PO4 (KDP); 2.5 The Computer-Assisted Molecular Design System for Searching New NLO Crystals
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3 Borate Nonlinear Optical Crystals for Frequency Conversion

Sommario/riassunto

This clear and self-contained review of the last four decades of research highlights in the hot field of nonlinear optical (NLO) crystals, particularly of borate-based ultraviolet and deep-ultraviolet NLO crystals, covers three major subjects: the structure-property relationship in borate crystals, the structural and optical characteristics of various promising borate crystals, and their fruitful applications in a wide range of scientific and technological fields. Edited by the discoverers and users of these optical borate crystals, this is a readily accessible reading for semiconductor, a