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Titolo	First-Principles and Machine Learning Study of Anharmonic Vibration and Dielectric Properties of Materials / / by Tomohito Amano
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Nota di contenuto	Chapter 1 Introduction -- Chapter 2 Density Functional Theory -- Chapter 3 Anharmonic Phonon Theory -- Chapter 4 Modern Theory and Machine Learning of Polarization -- Chapter 5 Dielectric Properties of Strongly Anharmonic TiO2 -- Chapter 6 Dielectric Properties of Liquid Alcohols and Its Polymers -- Chapter 7 Conclusion.
Sommario/riassunto	The book presents the author's development of two first-principles methods to calculate dielectric properties of materials based on anharmonic phonon and machine learning, and demonstrates an in-depth analysis of anharmonic crystals and molecular liquids. The

anharmonic phonon method, combined with Born effective charges, is useful to study dielectric properties of crystals. The recently developed self-consistent phonon theory (SCPH) enables accurate simulations in strongly anharmonic materials. The author reveals that the combination of SCPH with the four-phonon scattering term accurately reproduces experimental spectra, and discusses how anharmonic phonon self-energies affect the dielectric properties. The second method is molecular dynamics with Wannier centers—the mass centers of Wannier functions. The author constructs a machine learning model that learns Wannier centers for each chemical bond from atomic coordinates to accurately predict the dipole moments. The developed method is, in principle, applicable to molecules of arbitrary size. Its effectiveness is demonstrated and the dielectric properties of several alcohols, including dipole moments, dielectric constants, and absorption spectra, are analyzed. This book benefits students and researchers interested in anharmonic phonons, machine learning, and dielectric properties.