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Sommario/riassunto

This book delves into the advanced concepts of electron density and its applications in Density Functional Theory (DFT). It covers various aspects of DFT, including computational techniques, chemical reactivity descriptors, and the impact of electron density on molecular properties. The text is a collaborative work by experts from the Birla Institute of Technology and other institutions, providing insights into the role of electron density in chemical processes and material properties. It is intended for researchers and students in chemistry and material science, offering both theoretical and practical knowledge in the field.