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Nota di bibliografia	Includes bibliographical references at the end of each chapters.
Nota di contenuto	Introduction -- Theoretical Background -- Methodological Developments -- Applications -- Conclusion and Outlook -- Computational Details -- Mathematical Derivations -- The Method of Imaginary Time Propagation.
Sommario/riassunto	This thesis provides a comprehensive description of methods used to compute the vibrational spectra of liquid systems by molecular dynamics simulations. The author systematically introduces theoretical basics and discusses the implications of approximating the atomic nuclei as classical particles. The strengths of the methodology are demonstrated through several different examples. Of particular interest are ionic liquids, since their properties are governed by strong and diverse intermolecular interactions in the liquid state. As a novel contribution to the field, the author presents an alternative route toward infrared and Raman intensities on the basis of a Voronoi tessellation of the electron density. This technique is superior to existing approaches regarding the computational resources needed. Moreover, this book presents an innovative approach to obtaining the magnetic moments and vibrational circular dichroism spectra of liquids, and demonstrates its excellent agreement with experimental reference data.

