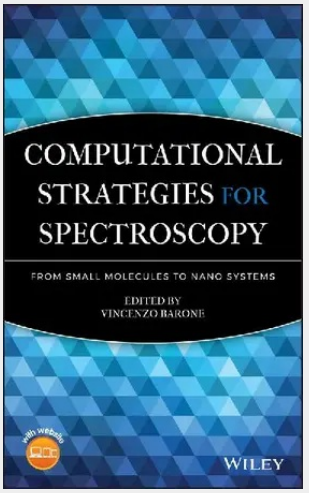
Barone

# Computational Strategies Spect




Computational spectroscopy is a rapidly evolving field that is becoming a versatile and widespread tool for the assignment of experimental spectra and their interpretation as related to chemical physical effects. This book is devoted to the most significant methodological contributions in the field, and to the computation of IR, UV-VIS, NMR and EPR spectral parameters with reference to the underlying vibronic and environmental effects. Each section starts with a chapter written by an experimental spectroscopist dealing with present challenges in the different fields; comprehensive coverage of conventional and advanced spectroscopic techniques is provided by means of dedicated chapters written by experts. Computational chemists, analytical chemists and spectroscopists, physicists, materials scientists, and graduate students will benefit from this thorough resource.

**Brings experimental data in alignment with sound theory in computational spectroscopy**

Computational spectroscopy is a rapidly evolving field that is becoming a versatile and widespread tool for the assignment of experimental spectra and their interpretation as related to chemical physical effects. Edited by a well-known researcher in the field, *Computational Strategies for Spectroscopy: From Small Molecules to Nano Systems* closes the gap between published computational results and sound theory to help scientists make accurate predictions and model more effectively in any application.

This book responds to the fact that the development of sophisticated experimental techniques poses correspondingly stringent requirements on the quality of the models employed to interpret spectroscopic results, and on the accuracy of the underlying chemical-physical descriptions. In such a complex scenario, theoretical studies can be extremely helpful.

Making modern computational strategies easily accessible to non-specialists as well as specialists, *Computational Strategies for Spectroscopy* presents a thorough overview of modern computational strategies for rotational. vibrational, electronic, and resonance spectroscopies covering a large interval of the electromagnetic spectrum, ranging from radiofrequencies to soft X-rays. The two sections of the book are devoted to:

- Transitions between electronic and spin states within a static framework
- Time-independent and time-dependent approaches to nuclear motions, with special reference to rotational, vibrational, and electronic spectroscopies

Dedicated chapters written by experts in the field give the reader a complete picture of the various spectroscopies from the general theoretical background to current challenges in the different fields. The stereo-electronic, vibrational, vibronic, and environmental effects on the overall spectral phenomena are analyzed for molecular systems ranging from small molecules to nano systems. Examples clearly illustrate the advantages and limitations of specific computational methods and models.

Providing the reader with a broad overview of the available computational approaches and their applicability, this carefully assembled resource will prove invaluable to computational chemists, analytical chemists and spectroscopists, physicists, materials scientists, and graduate students alike.

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