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Nota di contenuto	Frontmatter -- Preface -- Contents -- List of Contributing Authors -- 1. Synthesis Meets Theory: Past, Present and Future of Rational Chemistry / Fianchini, Mauro -- 2. Close Contacts at the interface: Experimental-computational synergies for solving complexity problems / Torras, Juan / Zanuy, David / Bertran, Oscar / Alemán, Carlos / Puiggali, Jordi / Turón, Pau / Revilla-López, Guillem -- 3. The Halogen bond: Nature and Applications / Costa, Paulo J. -- 4. Effect of protonation, composition and isomerism on the redox properties and Electron (de)localization of classical polyoxometalates / López, Xavier -- 5. Modeling of Azobenzene-Based Compounds / Marturano, V. / Ambrogi, V. / Bandeira, N. A. G. / Tylkowski, B. / Giamberini, M. / Cerruti, P. -- 6. Gas-Phase High-Resolution molecular spectroscopy for Lav molecules / Gulaczyk, Iwona -- 7. Computer Analysis of Potentiometric data of complexes formation in the Solution / Jastrzab, Renata / Kaczmarek, Magorzata T. / Tylkowski, Bartosz / Odani, Akira -- 8. Reactive Extraction at Liquid-Liquid Systems / Wieszczycka, Karolina -- 9. Membrane Processes / Staszak, Katarzyna -- 10. The Problem of fouling in submerged membrane bioreactors - Model Validation and experimental evidence / Tsibranska, Irene / Vlaev, Serafim / Tylkowski, Bartosz -- 11. Applicability of DFT model in reactive distillation / Staszak, Maciej -- Index

Sommario/riassunto

This book gives an overview of recent integrated and inter-disciplinary approaches between chemical experiment and theory in a variety of fields, from polymer science to materials chemistry and ranging from the design of tailored properties to catalysis and reactivity, building on the well-established success of Density Functional Theory as the foremost quantum chemical method to provide qualitative and quantitative interpretation of results from the chemical laboratory. The combination of several characterization techniques with an understanding at the molecular level of chemical and physical phenomena are the main focal point of the subject matter.
