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| Note generali | Description based upon print version of record. |
| Nota di bibliografia | Includes bibliographical references at the end of each chapters. |
| Nota di contenuto | From the Contents: The Second Order Ehrenfest Method A Practical CASSCF Approach to Coupled Electron-Nuclear Dynamics -- Anchoring the Potential Energy Surface for the Br + H2O HBr + OH Reaction -- Isaiah Shavitt - Computational Chemistry Pioneer.-Comparison of one-dimensional and quasi-one-dimensional Hubbard models from the variational two-electron reduced-density-matrix method -- Steric and electrostatic effects on photoisomerization dynamics using QM/MM ab initio multiple spawning. |
| Sommario/riassunto | In this Festschrift dedicated to the late Isaiah Shavitt (1925-2012) , selected researchers in theoretical chemistry present research highlights on major developments in the field. Originally published in the journal Theoretical Chemistry Accounts, these outstanding contributions are now available in a hardcover print format, as well as a special electronic edition. This volume provides valuable content for all researchers in theoretical chemistry, and will especially benefit those research groups and libraries with limited access to the journal. |

