1. Record Nr. UNIORUON00172642

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| Titolo | Bibliothèque des chercheurs et des curieux |
| Pubbl/distr/stampa | Paris, : Librairie Delagrave |
| Lingua di pubblicazione | Non definito |
| Formato | Materiale a stampa |
| Livello bibliografico | Collezione |

2. Record Nr. UNINA9910254030203321

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| Titolo | Péter R. Surján : a Festschrift from theoretical chemistry accounts / / edited by Ágnes Szabados, Mihály Kállay, Péter G. Szalay |
| Pubbl/distr/stampa | Berlin, Heidelberg : , : Springer Berlin Heidelberg : , : Imprint : Springer, , 2016 |
| ISBN | 3-662-49825-1 |
| Edizione | [1st ed. 2016.] |
| Descrizione fisica | 1 online resource (259 p.) |
| Collana | Highlights in Theoretical Chemistry, , 2194-8666 ; ; 12 |
| Disciplina | 541 |
| Soggetti | Chemistry, Physical and theoretical<br>Atomic structure<br>Molecular structure<br>Theoretical and Computational Chemistry<br>Atomic/Molecular Structure and Spectra<br>Physical Chemistry |
| Lingua di pubblicazione | Inglese |
| Formato | Materiale a stampa |
| Livello bibliografico | Monografia |
| 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 content: Preface -- Local random phase approximation with projected oscillator orbitals -- Orthogonality-constrained Hartree–Fock and perturbation theory for high-spin open-shell excited states -- On the non-integer number of particles in molecular system domains: treatment and description.-Spin contamination and noncollinearity in general complex Hartree–Fock wave functions.-Partial-wave decomposition of the ground-state wavefunction of the two-electron |

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| | harmonium atom.-Use of graphics processing units for efficient evaluation of derivatives of exchange integrals by means of Fourier transformation. |
| Sommario/riassunto | In this Festschrift dedicated to the 60th birthday of Péter R. Surján, 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. |