

1. Record Nr.	UNINA9910298533203321
Titolo	8th Congress on Electronic Structure : Principles and Applications (ESPA 2012) : a conference selection from theoretical chemistry accounts // Juan J. Novoa, Manuel F. Ruiz-Lopez, volume editors ; with contributions from Manuel Alcamí [and eighty-four others]
Pubbl/distr/stampa	Heidelberg, Germany : , : Springer, , 2014
ISBN	3-642-41272-6
Edizione	[1st ed. 2014.]
Descrizione fisica	1 online resource (vi, 230 pages) : illustrations (chiefly color)
Collana	Highlights in Theoretical Chemistry, , 2194-8666 ; ; 5
Disciplina	530.4 541.2
Soggetti	Electronic structure Chemistry, Physical and theoretical
Lingua di pubblicazione	Inglese
Formato	Materiale a stampa
Livello bibliografico	Monografia
Note generali	"ISSN: 2194-8666." "ISSN: 2194-8674 (electronic)."
Nota di bibliografia	Includes bibliographical references.
Nota di contenuto	From the Contents: Analysis of the origin of lateral interactions in the adsorption of small organic molecules on oxide surfaces -- First-principles study of structure and stability in Si-C-O-based materials -- A time-dependent DFT/molecular dynamics study of the proton-wire responsible for the red fluorescence in the LSSmKate2 protein -- Preface to the ESPA-2012 special issue.
Sommario/riassunto	This volume collects research findings presented at the 8th Edition of the Electronic Structure: Principles and Applications (ESPA-2012) International Conference, held in Barcelona, Spain on June 26-29, 2012. The contributions cover research work on methods and fundamentals of theoretical chemistry, chemical reactivity, bimolecular modeling, and materials science. Originally published in the journal Theoretical Chemistry Accounts, these outstanding papers 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.

