

1. Record Nr.	UNINA9910141258203321
Autore	Weinhold Frank <1941->
Titolo	Discovering chemistry with natural bond orbitals [[electronic resource] /] / Frank Weinhold, Clark R. Landis
Pubbl/distr/stampa	Hoboken, N.J., : Wiley, 2012
ISBN	1-280-77867-9 9786613689061 1-118-22919-3 1-118-22910-X 1-118-22916-9
Descrizione fisica	1 online resource (350 p.)
Classificazione	SCI013050
Altri autori (Persone)	LandisClark R. <1956->
Disciplina	541/.28
Soggetti	Chemical bonds Molecular orbitals
Lingua di pubblicazione	Inglese
Formato	Materiale a stampa
Livello bibliografico	Monografia
Note generali	Includes index.
Nota di contenuto	1. Getting started -- 2. Electrons in atoms -- 3. Atoms in molecules -- 4. Hybrids and bonds in molecules -- 5. Resonance delocalization corrections -- 6. Steric and electrostatic effects -- 7. Nuclear and electronic spin effects -- 8. Coordination and hyperbonding -- 9. Intermolecular interactions -- 10. Transition state species and chemical reactions -- 11. Excited state chemistry.
Sommario/riassunto	"This book is about chemical bonds, their intrinsic energies and the corresponding dissociation energies which are relevant in reactivity problems; it is the first book to detail relatively uncomplicated but physically meaningful approaches to molecular properties, an area important to help understand chemical principles and predict chemical properties. The primary goal of this book is to enable students to gain proficiency in using the NBO program to re-express complex many-electron wavefunctions in terms of intuitive chemical concepts and orbital imagery, with minimal distractions from underlying mathematical or programming details"--