1. Record Nr. UNINA9910811579803321

Titolo	Metallic systems : a quantum chemist's perspective / / edited by Thomas C. Allison, Orkid Coskuner, Carlos A. Gonzalez
Pubbl/distr/stampa	Boca Raton, Fla., : CRC Press, 2011 Boca Raton, Fla. : , : CRC Press, , 2011
ISBN	0-429-13823-7 1-4200-6086-4
Edizione	[1st ed.]
Descrizione fisica	1 online resource (412 p.)
Altri autori (Persone)	AllisonThomas Clayton CoskunerOrkid GonzalezCarlos A
Disciplina	669/.94
Soggetti	Metals Quantum 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.
Nota di contenuto	Front Cover; Contents; Introduction; Contributors; Chapter 1: First Principles DFT Studies of Metal-Based Biological and Biomimetic Systems; Chapter 2: Structural and Thermodynamic Studies of a-Synuclein Proteins Related to Parkinson's Disease: Impact of Aqueous Solut; Chapter 3: Carbohydrate and Trivalent Iron Ion Interactions in the Gas Phase and in Aqueous Solution; Chapter 4: Aqueous Solutions of Metal Ions; Chapter 5: Structure of Liquid Metal Surfaces: A First Principles Perspective Chapter 6: Some Practical Considerations for Density Functional Theory Studies of Chemistry at Metal SurfacesChapter 7: Computational Investigations of Metal Oxide Surfaces; Chapter 8: Tight Binding Methods for Metallic Systems; Chapter 9: Density Functional Calculations of Metal Clusters: Structure, Dynamics, and Reactivity; Chapter 10: Density Functional Theory Calculations on Cobalt and Platinum Transition Metal Clusters; Chapter 11: Exploring the Borderland between Physics and Chemistry: Theoretical Methods in the Study of Atomic Clusters; Back Cover
Sommario/riassunto	Metallic systems are ubiquitous in daily life. They play key roles, for

example, in the chemistry of many biomolecules, ionic solutions, nanoparticles, and catalytic processes. They may be in solid, liquid, or gaseous form. The interactions of other molecules with metal surfaces are of considerable importance. Each of these topics is addressed in Metallic Systems. As we have entered the age where theoretical approaches are sufficiently mature to complement and guide experiments in many areas, an understanding of the theoretical tools and approaches to studying metallic syst