Record Nr. UNINA9910457254303321 Chemical bonding at surfaces and interfaces [[electronic resource] /] / **Titolo** edited by Anders Nilsson, Lars G.M. Pettersson and Jens K. Norskov Amsterdam;; Oxford,: Elsevier, 2008 Pubbl/distr/stampa **ISBN** 1-281-03451-7 9786611034511 0-08-055191-2 Descrizione fisica 1 online resource (533 p.) Altri autori (Persone) NilssonAnders PetterssonLars NorskovJ. K (Jens K.) Disciplina 541.224 Soggetti Chemical bonds Surface chemistry Electronic books. 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 and index. Front Cover; Chemical Bonding at Surfaces and Interfaces; Copyright Nota di contenuto Page: Table of Contents: Preface: Chapter 1 Surface Structure: 1. Why surface structure?; 2. Methods of surface adsorbate structure determination: 2.1. General comments: 2.2. Electron scattering: 2.3. Xray scattering; 2.4. Ion scattering; 2.5. Spectroscopic methods and scanning probe microscopy; 3. Adsorbate-induced surface reconstruction; 4. Molecular adsorbates - local sites, orientations and intramolecular bondlengths; 4.1. General issues and the case of CO on metals; 4.2. Simple hydrocarbons on metals 4.3. Carboxylates on metals4.4. Other substrates: molecules on Si; 5. Chemisorption bondlengths; 5.1. Metal surfaces; 5.2. Oxide surfaces; 6. Conclusions; Chapter 2 Adsorbate Electronic Structure and Bonding on Metal Surfaces; 1. Introduction; 2. Probing the electronic structure; 3. Adsorbate electronic structure and chemical bonding; 4. Adsorbate systems; 5. Radical atomic adsorption; 5.1. The electronic structure of N on Cu(100); 5.2. Chemical bonding of atomic adsorbates; 6. Diatomic

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Sommario/riassunto

Molecular surface science has made enormous progress in the past 30 years. The development can be characterized by a revolution in fundamental knowledge obtained from simple model systems and by an explosion in the number of experimental techniques. The last 10 years has seen an equally rapid development of quantum mechanical modeling of surface processes using Density Functional Theory (DFT). Chemical Bonding at Surfaces and Interfaces focuses on phenomena and concepts rather than on experimental or theoretical techniques. The aim is to provide the common basis for describing the i