1. Record Nr. UNINA9910454944003321

Titolo	Solvent effects and chemical reactivity [[electronic resource] /] / edited by Orlando Tapia and Juan Bertran
Pubbl/distr/stampa	Dordrecht ; ; Boston, : Kluwer Academic Publishers, c1996
ISBN	1-280-20541-5 9786610205417 0-306-46931-6
Edizione	[1st ed. 2002.]
Descrizione fisica	1 online resource (390 p.)
Collana	Understanding chemical reactivity ; ; v. 17
Altri autori (Persone)	TapiaOrlando <1938-> BertranJ <1931-> (Juan)
Disciplina	541.3/4
Soggetti	Reactivity (Chemistry) Solution (Chemistry) Solvation Solvents 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.
Nota di contenuto	Continuum Solvation Models -- Theoretical Basis for the Treatment of Solvent Effects in the Context of Density Functional Theory -- Monte Carlo Simulations of Chemical Reactions in Solution -- Computer Simulation for Chemical Systems: from Vacuum to Solution -- Crossing the Transition State in Solution -- Valence Bond Multistate Approach to Chemical Reactions in Solution -- Quantum Theory of Solvent Effects and Chemical Reactions.
Sommario/riassunto	This book gathers original contributions from a selected group of distinguished researchers that are actively working in the theory and practical applications of solvent effects and chemical reactions. The importance of getting a good understanding of surrounding media effects on chemical reacting system is difficult to overestimate. Applications go from condensed phase chemistry, biochemical reactions in vitro to biological systems in vivo. Catalysis is a phenomenon produced by a particular system interacting with the reacting subsystem. The result may be an increment of the chemical

rate or sometimes a decreased one. At the bottom, catalytic sources can be characterized as a special kind of surrounding medium effect. The materials involving in catalysis may range from inorganic components as in zeolites, homogenous components, enzymes, catalytic antibodies, and ceramic materials. . With the enormous progress achieved by computing technology, an increasing number of models and phenomenological approaches are being used to describe the effects of a given surrounding medium on the electronic properties of selected subsystem. A number of quantum chemical methods and programs, currently applied to calculate in vacuum systems, have been supplemented with a variety of model representations. With the increasing number of methodologies applied to this important field, it is becoming more and more difficult for non-specialist to cope with theoretical developments and extended applications. For this and other reasons, it is was deemed timely to produce a book where methodology and applications were analyzed and reviewed by leading experts in the field.

2. Record Nr. UNISA996465806703316

Titolo	Database: Enterprise, Skills and Innovation [[electronic resource]] : 22nd British National Conference on Databases, BNCOD 22, Sunderland, UK, July 5-7, 2005, Proceedings / / edited by Mike Jackson, David Nelson, Sue Stirk
Pubbl/distr/stampa	Berlin, Heidelberg : , : Springer Berlin Heidelberg : , : Imprint : Springer, , 2005
ISBN	3-540-31677-9 3-540-26973-8
Edizione	[1st ed. 2005.]
Descrizione fisica	1 online resource (XII, 185 p.)
Collana	Information Systems and Applications, incl. Internet/Web, and HCI ; ; 3567
Disciplina	005.74
Soggetti	Database management Information storage and retrieval Application software Database Management Information Storage and Retrieval Information Systems Applications (incl. Internet)
Lingua di pubblicazione	Inglese

Formato	Materiale a stampa
Livello bibliografico	Monografia
Note generali	Bibliographic Level Mode of Issuance: Monograph
Nota di bibliografia	Includes bibliographical references and index.
Nota di contenuto	Invited Paper -- Databases in Grid Applications: Locality and Distribution -- Spatio-temporal Databases -- Spatial Hierarchies and Topological Relationships in the Spatial MultiDimER Model -- Multidimensional Structures Dedicated to Continuous Spatiotemporal Phenomena -- TimeERplus: A Temporal EER Model Supporting Schema Changes -- Data Integration and Information Retrieval -- Semantically Rich Materialisation Rules for Integrating Heterogeneous Databases -- Answering Queries Using Views in the Presence of Functional Dependencies -- LAX: An Efficient Approximate XML Join Based on Clustered Leaf Nodes for XML Data Integration -- Exploitation of Referential Integrity Constraints for Efficient Update of Data Warehouse Views -- Correlation-Based Data Broadcasting in Wireless Networks -- Hierarchical Group-Based Sampling -- Using Schema Transformation Pathways for Data Lineage Tracing -- XML -- XDGL: XPath-Based Concurrency Control Protocol for XML Data -- Updating XML Using Object-Relational Database -- Applied Information Management -- Image Retrieval Using Weighted Color Co-occurrence Matrix -- Street Address Correction Based on Spelling Techniques -- Personalising Patient Information in the Real World -- Republishers in a Publish/Subscribe Architecture for Data Streams.
Sommario/riassunto	The British National Conference on Databases (BNCOD) was established in 1980 as a forum for research into the theory and practice of databases. The original conference in the series took place at the University of Aberdeen. To be precise, this conference was in fact entitled ICOD which stood for International Conference on Databases. It was the intention, when the series began, that an ICOD would take place every two years, whilst a BNCOD would run in the years in between. As the record shows ICOD was only held in 1980 and 1983. The more junior conference has managed to acquire a lifetime much longer than that of its senior relative! If truth wereknown,however, BNCOD has,overthe years,growninto ICOD and although the conference is still titled “British National,” it is, in fact, an international conference that takes place on a yearly basis. Proof of this can be obtained simply by looking at the table of contents of these proceeding which clearlyshowthatthe majorityofpaperspresentedatthis year’ sconferencecame from contributors whose a?liations are outside the UK. Despitetherangeofpapersono?er,BNCODstillretainsitsuniquelyBritish ?avor. The Programme Committee is drawn from UK academics and the c- ference is always held at a British university (or in earlier years a polytechnic!).