

1. Record Nr.	UNINA9910139545203321
Titolo	Modeling solvent environments [[electronic resource] ] : applications to simulations of biomolecules // edited by Michael Feig
Pubbl/distr/stampa	Weinheim, : Wiley-VCH Verlag GmbH, c2010
ISBN	1-282-47232-1 9786612472329 3-527-62925-4 3-527-62926-2
Descrizione fisica	1 online resource (336 p.)
Altri autori (Persone)	FeigMichael
Disciplina	541.3482011
Soggetti	Solvents Biomolecules 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	Modeling Solvent Environments: Applications to Simulations of Biomolecules; Contents; Preface; List of Contributors; 1: Biomolecular Solvation in Theory and Experiment; 1.1 Introduction; 1.2 Theoretical Views of Solvation; 1.2.1 Equilibrium Thermodynamics of Solvation; 1.2.2 Radial Distribution Functions; 1.2.3 Integral Equation Formalisms; 1.2.4 Kirkwood-Buff Theory; 1.2.5 Kinetic Effects of Solvation; 1.3 Computer Simulation Methods in the Study of Solvation; 1.3.1 Molecular Dynamics and Monte Carlo Simulations; 1.3.2 Water Models; 1.3.3 Solvent Structure and Dynamics from Simulations 1.3.4 Free Energy Simulations1.4 Experimental Methods in the Study of Solvation; 1.4.1 X-Ray/Neutron Diffraction and Scattering; 1.4.2 Nuclear Magnetic Relaxation; 1.4.3 Optical Spectroscopy; 1.4.4 Dielectric Dispersion; 1.5 Hydration of Proteins; 1.5.1 Protein Folding and Peptide Conformations in Aqueous Solvent; 1.5.2 Molecular Properties of Water Near Protein Surfaces; 1.5.3 Water Molecules at Protein-Ligand and Protein-Protein Interfaces; 1.6 Hydration of Nucleic acids; 1.7 Non-Aqueous Solvation; 1.7.1 Alcohols; 1.7.2 Urea; 1.7.3 Glycerol; 1.8 Summary; References

2: Model-Free "Solvent Modeling" in Chemistry and Biochemistry Based on the Statistical Mechanics of Liquids  
2.1 Introduction; 2.2 Outline of the RISM and 3D-RISM theories; 2.3 Partial Molar Volume of Proteins; 2.4 Detecting Water Molecules Trapped Inside Protein; 2.5 Selective Ion Binding by Protein; 2.6 Water Molecules Identified as a Substrate for Enzymatic Hydrolysis of Cellulose; 2.7 CO Escape Pathway in Myoglobin; 2.7.1 Effect of Protein Structure on the Distribution of Xe; 2.7.2 Partial Molar Volume Change Through the CO Escape Pathway of Myoglobin; 2.8 Perspective; References

3: Developing Force Fields From the Microscopic Structure of Solutions: The Kirkwood-Buff Approach  
3.1 Introduction; 3.2 Biomolecular Force Fields; 3.3 Examples of Problems with Current Force Fields; 3.4 Kirkwood-Buff Theory; 3.5 Applications of Kirkwood-Buff Theory; 3.6 The General KBFF Approach; 3.7 Technical Aspects of the KBFF Approach; 3.8 Results for Urea and Water Binary Solutions; 3.9 Preferential Interactions of Urea; 3.10 Conclusions and Future Directions; Acknowledgments; References

4: Osmolyte Influence on Protein Stability: Perspectives of Theory and Experiment  
4.1 Introduction  
4.2 Denaturing Osmolytes  
4.2.1 Does Urea Weaken Water Structure?;  
4.2.2 Effect of Urea on Hydrophobic Interactions; 4.2.3 Direct Interaction of Urea with Proteins; 4.3 Protecting Osmolytes; 4.3.1 Do Protecting Osmolytes Increase Water Structure?; 4.3.2 Effect of Protecting Osmolytes on Hydrophobic Interactions; 4.4 Mixed Osmolytes; 4.5 Conclusions; Acknowledgments; References

5: Modeling Aqueous Solvent Effects through Local Properties of Water;  
5.1 The Role of Water and Cosolutes on Macromolecular Thermodynamics; 5.2 Forces Induced by Water in Aqueous Solutions  
5.2.1 Interactions in Water-Accessible Regions of Proteins

---

Sommario/riassunto

A comprehensive view of the current methods for modeling solvent environments with contributions from the leading researchers in the field. Throughout, the emphasis is placed on the application of such models in simulation studies of biological processes, although the coverage is sufficiently broad to extend to other systems as well. As such, this monograph treats a full range of topics, from statistical mechanics-based approaches to popular mean field formalisms, coarse-grained solvent models, more established explicit, fully atomic solvent models, and recent advances in applying ab initio me

---

2. Record Nr.	UNINA9910172239703321
Autore	Mazumdar Dipak <1932->
Titolo	Globalization, labor markets and inequality in India // Dipak Mazumdar and Sandip Sarkar
Pubbl/distr/stampa	London ; ; New York, : Routledge Ottawa, ON, : International Development Research Centre, 2008
ISBN	1-00-306095-1 1-00-011569-0 1-000-15496-3 1-000-11569-0 1-003-06095-1 1-281-28891-8 9786611288914 1-55250-373-9
Edizione	[1st.]
Descrizione fisica	1 online resource (380 p.)
Collana	Routledge studies in the growth economies of Asia (2005) ; ; 79
Altri autori (Persone)	SarkarSandip <1961->
Disciplina	331.120954
Soggetti	Globalization - Economic aspects - India Labor market - India Equality - India India Economic conditions India Foreign economic relations
Lingua di pubblicazione	Inglese
Formato	Materiale a stampa
Livello bibliografico	Monografia
Note generali	Previously issued in print: 2008. <P>1. Introduction: An Overview of Globalization, Reforms and Macro-Economic Developments in India <STRONG>Part 1: Trends in Poverty, Inequality, Employment and Earnings </STRONG>2. Poverty, Growth and Inequality in the Pre- and Post-Reform Periods and the Patterns of Urbanization in India: An Analysis for All-India and the Major States 3. Trends in Employment and Earnings 1983-2000 4. Accounting for the Decline in Labor Supply in the Nineties <STRONG>Part 2: Regional Dimensions</STRONG> 5. Some Implications of Regional Differences in Labor Market Outcomes in India <EM>Ahmad Ahsan and Carmen Pages</EM> 6. Trend in Regional Disparities in Poverty, Incidence: An Analysis based on NSS Regions <STRONG>Part 3: Employment and Earnings in the Major Sectors</STRONG> 7. Agricultural Productivity,

Off-Farm Employment and Rural Poverty: The Problem of Labor Absorption in Agriculture 8. Employment Elasticity in Organized Manufacturing in India 9. Dualism in Indian Manufacturing: Causes and Consequences 10. Growth of Employment and Earnings in the Tertiary Sector <STRONG>Part 4: Labor Market Institutions</STRONG> 11. Regulations, Enforcement and Adjudication in Indian Labor Markets: Origins, Consequences and the Way Forward <EM>Ahmad Ahsan, Carmen Pages and Tirthankar Roy</EM> 12. Strengthening Employment and Social Security for Unorganized Workers <EM>Philip O'Keefe </EM> 13. Epilogue. Conclusions</P>

---

Nota di bibliografia

Includes bibliographical references (p. [342]-351) and index.

---

Nota di contenuto

Contents; List of figures; List of tables; List of maps; 1 Introduction: an overview of globalization, reforms and macro-economic developments in India; PART I: Trends in poverty, inequality, employment and earnings; PART II: Regional dimensions; PART III: Employment and earnings in the major sectors; PART IV: Labor-market institutions; PART V: Epilogue and conclusions; Notes; References; Index

---

Sommario/riassunto

India started on a program of reforms, both in its external and internal aspects, sometime in the mid-eighties and going on into the nineties. While the increased exposure to world markets (globalization') and relaxation of domestic controls has undoubtedly given a spurt to the GDP growth rate, its impact on poverty, inequality and employment have been controversial. This book examines in detail these aspects of post-reform India and discerns the changes and trends which these new developments have created. Providing an original analysis of unit-level data available from the quinquennial National Sample Surveys, the Annual Surveys of Industries and other basic data sources, the authors analyse and compare the results with other pieces of work in the literature. As well as describing the overall situation for India, the book highlights regional differences, and looks at the major industrial sectors such as agriculture, manufacturing and tertiary services. The important topic of labor market institutions - both for the formal or organized and the unorganized sectors - is considered and the possible adverse effect on employment growth of the regulatory labor framework is examined carefully. Since any reform of this framework must go hand in hand with better state intervention in the informal sector to have any chance of acceptance politically, some of the major initiatives in this area are critically explored. Overall, this book will be of great interest to development economists, labour economists and specialists in South Asian Studies.

---