

1. Record Nr.	UNINA9910458172603321
Titolo	Recent advances in density functional methods . Part III [[electronic resource] /] / edited by Vincenzo Barone, Alessandro Bencini, Piercarlo Fantucci
Pubbl/distr/stampa	Singapore ; ; River Edge, N.J., : World Scientific, 2002
ISBN	981-277-816-0
Descrizione fisica	1 online resource (432 p.)
Collana	Recent advances in computational chemistry ; ; v. 1
Altri autori (Persone)	BaroneVincenzo BenciniAlessandro <1951-> FantucciPiercarlo
Disciplina	542.85
Soggetti	Density functionals Quantum chemistry Electronic structure 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	CONTENTS ; Preface ; Theoretical Study of the Transition-Metal Silonyl Complexes M-SiO and M-(SiO) <sub>2</sub> : M = Cu Ag or Au ; 1 Introduction ; 2 Results and Discussion ; 3 Concluding Remarks ; References Local Relaxation for Mn <sup>2+</sup> and Fe <sup>3+</sup> Impurities in Fluoroperovskites: Density Functional Study 1 Introduction ; 2 Theoretical ; 3 Results and discussion ; 4 Acknowledgement ; 5 References Theoretical Exploration of Single and Multi State Femtosecond Nuclear Dynamics of Small Metallic Clusters Using the DF Method 1 Introduction ; 2 Computational ; 3 Results and Discussion of Dynamics of Li <sup>+</sup> <sub>9</sub> Cluster ; 4 Multi State Dynamics of Ag <sup>4-</sup> /Ag <sub>4</sub> /Ag <sub>4</sub> <sup>+</sup> ; 5 Conclusion ; References Applications of Density Functional Theory in Solid State Chemistry

1 Introduction ; 2 Spin States in Bimetallic Clusters: Effects on Structure and Energetics ; 3 Electronic Structure Magnetic Ordering in BEDT-TTF Charge Transfer Salts ; 3.1 Isolated Molecules ; 3.2 Periodic Systems ; 4 Peroxy Species: Environmental and Electron Correlation Effects ; 4.1 Crystalline Ionic Peroxide Materials ; 4.2 Peroxy Species in Bulk Zeolites and Related Materials ; 5. Conclusion ; 6 Acknowledgements ; References ; A Hybrid Functional for the Exchange-Correlation Kernel in Time-Dependent Density Functional Theory

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Sommario/riassunto

In the last few years, much attention has been given by theoretical chemists to the development of more accurate model functionals and faster computational techniques including excited electronic states. The 8th International Conference on the Applications of Density Functional Theory to Chemistry and Physics, held in Rome, Italy, on 6-10 September 1999, gathered chemists and physicists to present and discuss state-of-the-art methodological developments and applications of density functional theory (DFT) to increasingly complex systems. The scientists shared their knowledge and experience in

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2. Record Nr.	UNINA9910792056503321
Titolo	Bioevaluation of world transport networks [[electronic resource] /] / edited by Andrew Adamatzky
Pubbl/distr/stampa	Singapore, : World Scientific, 2012
ISBN	1-299-28105-2 981-4407-04-6
Descrizione fisica	1 online resource (368 p.)
Altri autori (Persone)	AdamatzkyAndrew
Disciplina	388.0113
Soggetti	Transportation - Computer simulation Transportation - Mathematical models Roads - History Plasmodium
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	Preface; Contents; Contributors; 1. Introduction Andrew Adamatzky; 1.1 Motorways; 1.2 Imitating road development; 1.3 Slime mould; 1.4 Physarum computing; 1.5 What the book is about; 2. Methods: how we conducted experiments and analysed their results Andrew Adamatzky; 2.1 Obtaining P. polycephalum; 2.2 Cultivation; 2.3 Experiments; 2.4 Physarum and motorway graphs; 2.5 Proximity graphs; 3. Trans- African highways Andrew Adamatzky and Anne Kayem; 3.1 Propagation from Cairo: three scenarios; 3.2 Protoplasmic networks of trans-African highways 3.3 Lubumbashi and Lusaka to Harare and Beira is the strongest link 3.4 Summary; 4. Tracing historical development of Australian highways Andrew Adamatzky and Mikhail Prokopenko; 4.1 Slime mould traces gold rush networking; 4.2 Physarum reconstructs the Gabriel graph; 4.3 Australian highways are a subnetwork of the Physarum network; 4.4 Famine and large-scale contamination; 4.5 Summary; 5. Belgian transport networks: redundancy and dissolution Andrew Adamatzky, Bernard De Baets and Wesley Van Dessel; 5.1 Bioessential motorways grow from Brussels 5.2 Physarum almost perfectly approximates Belgian motorways 5.3

Minimum spanning tree is not a subgraph of motorway graph; 5.4 Dissolution: snelwegen or autoroutes?; 5.5 Doel nuclear power plant and other sources of contamination; 5.6 Summary; 6. Brazilian highways from slime mould's point of view Andrew Adamatzky and Pedro P. B. de Oliveira; 6.1 Slime mould makes more highways; 6.2 Comparing with proximity graph; 6.3 Physarum and Angra nuclear power plant; 6.4 Summary; 7. Trans-Canada slimeways: from coast to coast to coast Andrew Adamatzky and Selim G. Akl; 7.1 Foraging from Toronto  
7.2 Physarum almost approximates Canadian highways 7.3 On optimality of Canadian highways; 7.4 Contamination from Bruce nuclear power station; 7.5 Summary; 8. Slime mould imitates highways in China Andrew Adamatzky, Xin-She Yang and Yu-Xin Zhao; 8.1 From Beijing to Urumqi; 8.2 Physarum graph belongs to motorway graph; 8.3 Slime and man-made networks vs proximity graphs; 8.4 Summary; 9. Schlauschleimer auf Autobahnen: the case of Germany Andrew Adamatzky and Theresa Schubert; 9.1 Germany colonised; 9.2 More connections in the west; 9.3 Reichsautobahn rediscovered; 9.4 Slimy proximity graphs  
9.5 Mass migration due to contamination 9.6 Summary; 10. Vie Physarale: Roman roads with slime mould Emanuele Strano, Andrew Adamatzky and Jeff Jones; 10.1 From Piacentia to Bononia and from Genua to Florenzia are missing; 10.2 Simulation: linking Bononia to Ariminum and Roma; 10.3 Summary; 11. Malaysian expressways: is there a logic behind them? Andrew Adamatzky, Zuwairie Ibrahim, Amar Faiz Zainal Abidin, Badaruddin Muhammad; 11.1 The coastal routes; 11.2 Strong chains and isolated cities; 11.3 Trees rooted in Rawan and Kuala Lumpur are minimal; 11.4 Contamination in Kuantan; 11.5 Summary  
12. Physarum narcotraficum: Mexican highways and slime mould Andrew Adamatzky, Genaro J. Martinez, Sergio V. Chapa- Vergara, Rene Asomoza-Palacio and Christopher R. Stephens

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## Sommario/riassunto

Slime mould *Physarum polycephalum* is a monstrous single cell well known for its task-solving abilities - solves computational geometry and logical problems, navigates robots and generates music. The slime mould could also build motorways, highways and expressways. It is used to analyse transport networks of Africa, Australia, Belgium, Brazil, Canada, China, Germany, Iberia, Italy, Malaysia, Mexico, The Netherlands, UK and USA. The largest cities are represented by oat flakes and the slime mould is inoculated in a capital. When all oat flakes are covered by the slime mould, the structure of the

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3. Record Nr.	UNINA9910864201303321
Autore	Randall R. Lor
Titolo	Metastatic Bone Disease : An Integrated Approach to Patient Care // edited by R. Lor Randall
Pubbl/distr/stampa	Cham : , : Springer International Publishing : , : Imprint : Springer, , 2024
ISBN	3-031-52001-7
Edizione	[2nd ed. 2024.]
Descrizione fisica	1 online resource (388 pages)
Disciplina	616.71
Soggetti	Orthopedics Oncology Orthopaedics
Lingua di pubblicazione	Inglese
Formato	Materiale a stampa
Livello bibliografico	Monografia
Nota di contenuto	Part I. The Problem -- Bone Metastases: Epidemiology and Societal Effect -- Part II. Biology of Metastases and Tissue of Origin Considerations -- Pathobiology of Osteolytic and Osteoblastic Bone Metastases -- Tissue Engineered Models to Study Bone Metastases -- Biology of Bone Cancer Pain -- Breast Cancer Bone Metastases -- Prostate Cancer Bone Metastases -- Lung Cancer Bone Metastases -- Kidney Cancer Bone Metastases -- Thyroid Cancer Bone Metastases -- Myeloma Bone Metastases -- Part III. Work-Up for Patients with Suspected Metastatic Bone Disease -- Evaluation of the Patient with Carcinoma of Unknown Origin Metastatic to Bone -- Biopsy Considerations -- Part IV. Medical Therapy for Metastatic Bone Disease -- Bisphosphonates, Denosumab, and Anabolic Agents in the Treatment of Metastatic Bone Disease -- Biotargeting in Metastatic Bone Disease -- Part V. Supportive Oncology for Metastatic Bone Disease -- Psychosocial Considerations for Patients with Metastatic Bone Disease -- Pain Management in Metastatic Bone Disease -- When Is Hospice Appropriate? The Role for Hospice in Palliating Patients with Bone Metastases -- PROs -- Part VI. Radiation Oncology -- Current and Emerging Modalities -- Part VII. Interventional Oncology for Metastatic Bone Disease -- Ablation and Cementation Technologies -- Part VIII. Principles of Orthopedic Surgical Oncology -- Issues Facing the

Established Metastatic Bone Disease Patient, Timing/Indications for Surgery -- Questions to Ask Your Medical Oncology Colleagues -- Consideration of the Temporal Relationship Between Surgery and Radiation Therapy -- Role of Surgery in Oligometastatic Disease -- Part IX. Specific Anatomic Considerations for Surgery -- Metastatic Bone Disease: Pelvis -- Metastatic Bone Disease: Femur -- Metastatic Bone Disease: Femur, Tibia -- Metastatic Bone Disease: Foot -- Metastatic Bone Disease: Humerus and Scapula -- Metastatic Bone Disease: Forearm, Hand -- Metastatic Bone Disease: Spine -- Part X. Emergent Surgical Technologies -- Intraoperative Imaging and Navigation -- Part XI. Putting It All Together -- Integrative Approach with the Patient in Mind: A Glance Forward.

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Sommario/riassunto

Skeletally related events make up approximately 20% of the cancer care economy. Advances in understanding the pathobiology and better biotargeted therapy and improved surgical technology are occurring continuously. Hundreds of thousands of patients are living longer with ever-increasing tumor burden, but patients can remain siloed in their care as they navigate across subspecialty treatments. This comprehensive text ties it all together around the patient, integrating all aspects of care. Providing an integrated approach to the diagnosis and management of patients with metastatic bone disease (MBD), this revised and expanded text combines discussion of the pathobiology of the disease with the latest oncological and orthopedic treatment modalities. After opening with an examination of the epidemiology and impact of MBD, the biology of bone metastases are discussed, along with considerations of the tissue of origin, evaluation, biopsy and medical therapy, including metabolic agents and biotargeting. The heart of the book presents oncological approaches (supportive, radiation and interventional) and principles of orthopedic surgical oncology, with subsequent chapters covering specific anatomy, from the pelvis to the lower extremity and the spine. Chapters on emerging surgical technology and future directions conclude the text. New to this edition are considerations around patient-reported outcomes. Utilizing the latest clinical evidence and treatment techniques, *Metastatic Bone Disease, Second Edition* is a standalone resource reflecting a comprehensive, patient-centric resource for all types of providers.

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