

1. Record Nr.	UNINA9910298309003321
Titolo	The Future of Dynamic Structural Science / / edited by Judith A.K. Howard, Hazel A. Sparkes, Paul R. Raithby, Andrei V. Churakov
Pubbl/distr/stampa	Dordrecht : , : Springer Netherlands : , : Imprint : Springer, , 2014
ISBN	94-017-8550-3
Edizione	[1st ed. 2014.]
Descrizione fisica	1 online resource (XVI, 284 p. 154 illus., 103 illus. in color.)
Collana	NATO Science for Peace and Security Series A: Chemistry and Biology, , 1874-6527
Disciplina	548/.8
Soggetti	Spectrum analysis Chemistry - Data processing Spectroscopy Computational Chemistry
Lingua di pubblicazione	Inglese
Formato	Materiale a stampa
Livello bibliografico	Monografia
Note generali	"Proceedings of the NATO Advanced Study Institute on The Future of Dynamic Structural Science: Links to Energy and Environmental Security and Early Detection of CBRN Agents, Erice, Italy, 30 May - 8 June, 2013."
Nota di contenuto	Single Crystal and Powder Methods for Structure Determination of Metastable Species -- Raman Crystallography, the Missing Link between Biochemical Reactions and Crystallography -- Structure and Dynamics from Time Resolved Absorption and Raman Spectroscopy -- Time and Space-Resolved Spectroscopy -- Dynamic X-Ray and Neutron Scattering: From Materials Synthesis and In-Situ Studies to Biology at High Pressure -- Dynamics of Mechanochemical Processes -- Measuring and Understanding Ultrafast Phenomena Using X-Rays -- Single-Crystal to Single-Crystal Solid-State Photochemistry -- Femtoseconds to Hours Structural Dynamics Investigations: What do the Different Time Scales tell us in Chemistry? -- Structure and Dynamics of Light-Excited States -- Direct Observation of Various Reaction Pathways in Crystalline State Photoreactions -- Time Resolved XAS Spectroscopy Probing Dynamic Species in Homogeneous Catalysis – Towards faster Methods Providing more Information -- Dynamical Aspects of Biomacromolecular Multi-Resolution Modelling Using the Ultra Scan Solution Modeler (US-SOMO) Suite -- Linking Diffraction,

XAFS and Spectroscopic Studies on Short Lived Species -- Structure Analyses of Unstable Reaction Intermediates Using the Technique of Acid-Base Complex or Polymorphic Crystal Formation -- Molecular Mechanisms of Light-Harvesting and Photo-Protection by Carotenoids Explaining Configurational Selections by Antenna and Reaction Centre Complexes -- Time-Resolved Macromolecular Crystallography in Practice at Bio CARS, Advanced Photon Source: from Data Collection to Structures of Intermediates -- Combining Single Crystal UV/Vis Spectroscopy and Diffraction to Structurally Characterise Intermediates and Monitor Radiation Damage -- Molecular Dynamics Probed by Short X-Ray Pulses from a Synchrotron.

Sommario/riassunto

This work focuses on complementary crystallographic and spectroscopic areas of dynamic structural science, from papers presented at the 46th NATO sponsored course in Erice, Sicily 2013. These papers cover a range of material from background concepts to more advanced material and represent a fully inter-disciplinary collection of the latest ideas and results within the field. They will appeal to practising or novice crystallographers, both chemical and biological, who wish to learn more about modern spectroscopic methods and convergent advances and hence vice versa for experimental and computational spectroscopists. The chapters refer to the latest techniques, software and results and each chapter is fully referenced. The volume provides an excellent starting point for new comers in the emerging, multi-disciplinary area of time resolved science.
