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Titolo	EPR of free radicals in solids I : trends in methods and applications // edited by Anders Lund, Masaru Shiotani
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Edizione	[2nd ed.]
Descrizione fisica	1 online resource (423 p.)
Collana	Progress in theoretical chemistry and physics, , 1567-7354 ; ; v. 24
Altri autori (Persone)	LundA (Anders) ShiotaniMasaru
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Nota di bibliografia	Includes bibliographical references and index.
Nota di contenuto	Continuous Wave EPR of Radicals in Solids (Anders Lund and Wei Liu) -- Pulse EPR of Paramagnetic Centers in Solid Phases (Marina Brustolon and Antonio Barbon) -- Dynamical Effects in CW and Pulsed EPR -- Deuterium Labeling Studies and Quantum Effects of Radicals in Solids (Nikolas- Ploutarch Benetis, Yuriy Dmitriev) -- XSophe - Sophe - XeprView and Molecular Sophe: Computer Simulation Software (Masaru Shiotani and Kenji Komaguchi) -- Suites for the Analysis of Continuous Wave and Pulsed EPR and ENDOR Spectra (Graeme R. Hanson, Christopher J. Noble, Simon Benson) -- The Calculation of the Hyperfine Coupling Tensors of Biological Radicals (Fuqiang Ban, James W. Gauld, Stacey D. Wetmore and Russell J. Boyd) -- Ab initio and Density Functional Calculations of Electronic g-Tensors for Organic Radicals (Martin Kaupp) -- Quantum Chemical Calculations of the Zero-Field Splitting Tensors for Organic Spin Multiplets (Kenji Sugisaki, Kazuo Toyota, Kazunobu Sato, Daisuke Shiomi, Masahiro Kitagawa and Takeji Takui).
Sommario/riassunto	EPR of Free Radicals in Solids: Trends in Methods and Applications, 2nd ed. presents a critical two volume review of the methods and applications of EPR (ESR) for the study of free radical processes and

structures in solids. Emphasis is on the progress made in the developments in EPR technology, in the application of sophisticated matrix isolation techniques and in the advancement in quantitative EPR that have occurred since the 1st edition was published. Improvements have been made also at the theoretical level, with the development of methods based on first-principles methods and their application to the calculation of magnetic parameters and to simulation of spectral shapes. Written by international leading experts in the field, EPR of Free Radicals in Solids I focuses on the trends in experimental and theoretical methods to extract structural and dynamical properties of radicals and spin probes in solid matrices by continuous wave (CW) and pulsed techniques. It presents simulation techniques and computer software for CW and pulsed EPR signals, and also studies quantum effects at low temperature. In this edition, the chapters dealing with quantum chemistry methods for the theoretical interpretation of hyperfine coupling tensors and g-tensors have been much extended and a new chapter on the calculation of zero-field splitting tensors has been added. This new edition is a valuable resource to both theoreticians and experimentalists active in research involving free radicals, as well as to students of advanced courses in physical chemistry, chemical physics, materials science, biophysics, biochemistry, and related fields. Written by international leading experts in the field, EPR of Free Radicals in Solids I focuses on the trends in experimental and theoretical methods to extract structural and dynamical properties of radicals and spin probes in solid matrices by continuous wave (CW) and pulsed techniques. It presents simulation techniques and computer software for CW and pulsed EPR signals, and also studies quantum effects at low temperature. In this edition, the chapters dealing with quantum chemistry methods for the theoretical interpretation of hyperfine coupling tensors and g-tensors have been much extended and a new chapter on the calculation of zero-field splitting tensors has been added. This new edition is a valuable resource to both theoreticians and experimentalists active in research involving free radicals, as well as to students of advanced courses in physical chemistry, chemical physics, materials science, biophysics, biochemistry, and related fields.

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