

1. Record Nr.	UNISA996466813803316
Titolo	Computer Simulation of Solids [[electronic resource] /] / edited by C. R. A. Catlow, W. C. Mackrodt
Pubbl/distr/stampa	Berlin, Heidelberg : , : Springer Berlin Heidelberg : , : Imprint : Springer, , 1982
ISBN	3-540-39347-1
Edizione	[1st ed. 1982.]
Descrizione fisica	1 online resource (XII, 325 p.)
Collana	Lecture Notes in Physics, , 0075-8450 ; ; 166
Disciplina	530.41
Soggetti	Condensed matter Condensed Matter Physics
Lingua di pubblicazione	Inglese
Formato	Materiale a stampa
Livello bibliografico	Monografia
Note generali	Bibliographic Level Mode of Issuance: Monograph
Nota di contenuto	Theory of simulation methods for lattice and defect energy calculations in crystals -- Theory and calculation of defect entropies -- Characteristic volumes of point defects in ionic crystals -- Free energy calculations for crystals -- Molecular dynamics simulations of crystalline ionic materials -- Ab initio cluster calculations for defects in the solid state -- Computational methods for the electronic structure of defects in insulators -- Interatomic potentials in solids -- Potentials in metals -- Interionic potentials in ionic solids -- Interatomic potentials in covalent and semi-covalent solids -- Defect calculations for ionic materials -- Point defect calculations in metals -- Defect calculations in semiconductors -- Computer modelling of complex and massively disordered crystalline solids -- Aspects of the chemistry of phyllosilicates and intercalation in vermiculites -- Aggregation and precipitation in alkali halides -- Computer simulation of fast ion conductors -- Computer simulation of ionic crystal surfaces -- Long range order in non-stoichiometric oxides.