1.	Record Nr.	UNISA996392476803316
	Autore	Cotton John <1584-1652.>
	Titolo	The way of life, or, Gods vvay and course, in bringing the soule into, keeping it in, and carrying it on, in the wayes of life and peace [[electronic resource]] : laid downe in foure severall treatises on foure texts of Scripture, viz. the pouring out of the spirit, on Zach. 12. 10, 11, &c., sins deadly wound, on Acts 2. 37., the Christians charge, on Prov. 4. 23., the life of faith, on Gal. 2. 19, 20 / / by ... John Cotton
	Pubbl/distr/stampa	London, : Printed by M.F. for L. Fawne and S. Gellibrand ..., 1641
	Descrizione fisica	[8], 481 p
	Soggetti	Christian life
	Lingua di pubblicazione	Inglese
	Formato	Materiale a stampa
	Livello bibliografico	Monografia
	Note generali	Reproduction of original in Huntington Library.
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2. Record Nr.	UNINA9910816354503321
Titolo	Electronic structure calculations on graphics processing units : from quantum chemistry to condensed matter physics / / Ross C. Walker and Andreas W. Goetz, editors
Pubbl/distr/stampa	West Sussex, England : , : Wiley, , 2016 ©2016
ISBN	1-118-67070-1 1-118-67071-X 1-118-67069-8
Descrizione fisica	1 online resource (448 p.)
Classificazione	SCI013050
Disciplina	621.39/96
Soggetti	Electronic structure - Computer simulation Electronic structure - Mathematical models Graphics processing units - Programming Mathematical physics
Lingua di pubblicazione	Inglese
Formato	Materiale a stampa
Livello bibliografico	Monografia
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Nota di bibliografia	Includes bibliographical references and index.
Nota di contenuto	Title Page; Copyright; Table of Contents; List of Contributors; Preface; Acknowledgments; Glossary; Abbreviations - Scientific; Abbreviations - Technical; Chapter 1: Why Graphics Processing Units; 1.1 A Historical Perspective of Parallel Computing; 1.2 The Rise of the GPU; 1.3 Parallel Computing on Central Processing Units; 1.4 Parallel Computing on Graphics Processing Units; 1.5 GPU-Accelerated Applications; References; Chapter 2: GPUs: Hardware to Software; 2.1 Basic GPU Terminology; 2.2 Architecture of GPUs; 2.3 CUDA Programming Model; 2.4 Programming and Optimization Concepts 2.5 Software Libraries for GPUs2.6 Special Features of CUDA-Enabled GPUs; References; Chapter 3: Overview of Electronic Structure Methods; 3.1 Introduction; 3.2 Hartree-Fock Theory; 3.3 Density Functional Theory; 3.4 Basis Sets; 3.5 Semiempirical Methods; 3.6 Density Functional Tight Binding; 3.7 Wave Function-Based Electron Correlation Methods; Acknowledgments; References; Chapter 4: Gaussian Basis Set Hartree-Fock, Density Functional Theory, and Beyond on GPUs; 4.1

Sommario/riassunto	"Electronic Structure Calculations on Graphics Processing Units: From Quantum Chemistry to Condensed Matter Physics provides an overview of computing on graphics processing units (GPUs), a brief introduction to GPU programming, and the latest examples of code developments and applications for the most widely used electronic structure methods. The book covers all commonly used basis sets including localized Gaussian and Slater type basis functions, plane waves, wavelets and real-space grid-based approaches. The chapters expose details on the calculation of two-electron integrals, exchange-correlation quadrature, Fock matrix formation, solution of the self-consistent field equations, calculation of nuclear gradients to obtain forces, and methods to treat excited states within DFT. Other chapters focus on semiempirical and correlated wave function methods including density fitted second order Moshlasser-Plesset perturbation theory and both iterative and perturbative single- and multireference coupled cluster methods. Electronic Structure Calculations on Graphics Processing Units: From Quantum Chemistry to Condensed Matter Physics presents an accessible overview of the field for graduate students and senior researchers of theoretical and computational chemistry, condensed matter physics and materials science, as well as software developers looking for an entry point into the realm of GPU and hybrid GPU/CPU programming for electronic structure calculations"--