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Titolo	Fascinating mathematical people [[electronic resource]] : interviews and memoirs / / Donald J. Albers and Gerald L. Alexanderson, editors ; with a foreword by Philip J. Davis
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Edizione	[Course Book]
Descrizione fisica	1 online resource (264 p.)
Altri autori (Persone)	AlbersDonald J. <1941-> AlexandersonGerald L DavisPhilip J
Disciplina	510.92/2
Soggetti	Mathematicians Electronic books.
Lingua di pubblicazione	Inglese
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Nota di contenuto	Frontmatter -- Contents -- Foreword / Davis, Philip J. -- Preface -- Acknowledgments -- Sources -- One. Lars V. Ahlfors / Albers, Donald J. -- Two. Tom Apostol / Albers, Donald J. -- Three. Harold M. Bacon / Alexanderson, Gerald L. -- Four. Tom Banchoff / Albers, Donald J. -- Five. Leon Bankoff / Alexanderson, Gerald L. -- Six. Alice Beckenbach -- Seven. Arthur Benjamin / Albers, Donald J. -- Eight. Dame Mary L. Cartwright / Tattersall, James / McMurran, Shawnee -- Nine. Joe Gallian / Haunsperger, Deanna -- Ten. Richard K. Guy / Albers, Donald J. / Alexanderson, Gerald L. -- Eleven. Fern Hunt / Henrion, Claudia -- Twelve. Dusa McDuff / Albers, Donald J. -- Thirteen. Donald G. Saari / Haunsperger, Deanna -- Fourteen. Atle Selberg / Alexanderson, Gerald L. -- Fifteen. Jean Taylor / Albers, Donald J. -- Sixteen. Philippe Tondeur / Albers, Donald J. -- Biographical. Notes -- Glossary -- Index
Sommario/riassunto	Fascinating Mathematical People is a collection of informal interviews and memoirs of sixteen prominent members of the mathematical community of the twentieth century, many still active. The candid portraits collected here demonstrate that while these men and women

vary widely in terms of their backgrounds, life stories, and worldviews, they all share a deep and abiding sense of wonder about mathematics. Featured here--in their own words--are major research mathematicians whose cutting-edge discoveries have advanced the frontiers of the field, such as Lars Ahlfors, Mary Cartwright, Dusa McDuff, and Atle Selberg. Others are leading mathematicians who have also been highly influential as teachers and mentors, like Tom Apostol and Jean Taylor. Fern Hunt describes what it was like to be among the first black women to earn a PhD in mathematics. Harold Bacon made trips to Alcatraz to help a prisoner learn calculus. Thomas Banchoff, who first became interested in the fourth dimension while reading a Captain Marvel comic, relates his fascinating friendship with Salvador Dalí and their shared passion for art, mathematics, and the profound connection between the two. Other mathematical people found here are Leon Bankoff, who was also a Beverly Hills dentist; Arthur Benjamin, a part-time professional magician; and Joseph Gallian, a legendary mentor of future mathematicians, but also a world-renowned expert on the Beatles. This beautifully illustrated collection includes many photographs never before published, concise introductions by the editors to each person, and a foreword by Philip J. Davis.Some images inside the book are unavailable due to digital copyright restrictions.

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Autore	Helgaker Trygve
Titolo	Molecular electronic-structure theory / / Trygve Helgaker, Poul Jorgensen, Jeppe Olsen
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ISBN	1-119-01957-5 1-119-01955-9 1-119-01956-7
Descrizione fisica	1 online resource (940 p.)
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Nota di contenuto	Cover; Title Page; Copyright; Contents; Preface; Overview; Programs used in the preparation of this book; 1 Second Quantization; 1.1 The Fock space; 1.2 Creation and annihilation operators; 1.2.1 Creation operators; 1.2.2 Annihilation operators; 1.2.3 Anticommutation relations; 1.3 Number-conserving operators; 1.3.1 Occupation-number operators; 1.3.2 The number operator; 1.3.3 Excitation operators; 1.4 The representation of one- and two-electron operators; 1.4.1 One-electron operators; 1.4.2 Two-electron operators; 1.4.3 The molecular electronic Hamiltonian 1.5 Products of operators in second quantization1.5.1 Operator products; 1.5.2 The canonical commutators; 1.6 First- and second-quantization operators compared; 1.7 Density matrices; 1.7.1 The one-electron density matrix; 1.7.2 The two-electron density matrix; 1.7.3 Density matrices in spin-orbital and coordinate representations; 1.8 Commutators and anti commutators; 1.9 Nonorthogonal spin orbitals; 1.9.1 Creation and annihilation operators; 1.9.2 One- and two-electron operators; 1.9.3 Biorthogonal operators; References; Further reading; Exercises; Solutions; 2 Spin in Second Quantization 2.1 Spin functions2.2 Operators in the orbital basis; 2.2.1 Spin-free

operators; 2.2.2 Spin operators; 2.2.3 Mixed operators; 2.3 Spin tensor operators; 2.3.1 Spin tensor operators; 2.3.2 Creation and annihilation operators; 2.3.3 Two-body creation operators; 2.3.4 Excitation operators; 2.3.5 Singlet excitation operators; 2.4 Spin properties of determinants; 2.4.1 General considerations; 2.4.2 Spin projection of determinants; 2.4.3 Total spin of determinants; 2.5 Configuration state functions; 2.6 The genealogical coupling scheme; 2.6.1 Representations of determinants and CSFs
2.6.2 Genealogical coupling2.6.3 Coupling coefficients; 2.6.4 An example: three electrons in three orbitals; 2.6.5 Completeness and orthonormality; 2.6.6 Transformations between determinant and CSF bases; 2.6.7 Genealogical coupling of operators; 2.7 Density matrices; 2.7.1 Orbital-density matrices; 2.7.2 Spin-density matrices; 2.7.3 Density functions; References; Further reading; Exercises; Solutions; 3 Orbital Rotations; 3.1 Unitary transformations and matrix exponentials; 3.1.1 Matrix exponentials; 3.1.2 Exponential representations of unitary matrices; 3.1.3 Special unitary matrices
3.1.4 Orthogonal matrices3.1.5 Evaluation of matrix exponentials; 3.1.6 Nonunitary transformations; 3.2 Unitary spin-orbital transfonnations; 3.2.1 Unitary matrix expansions of creation and annihilation operators; 3.2.2 Exponential unitary transfonnations of the elementary operators; 3.2.3 Exponential unitary transfonnations of states in Fock space; 3.3 Symmetry-restricted unitary transfonnations; 3.3.1 The need for symmetry restrictions; 3.3.2 Symmetry restrictions in the spin-orbital basis; 3.3.3 Symmetry restrictions in the orbital basis; 3.4 The logarithmic matrix function
3.4.1 Definition of the logarithmic matrix function

Sommario/riassunto

Ab initio quantum chemistry has emerged as an important tool in chemical research and is appliced to a wide variety of problems in chemistry and molecular physics. Recent developments of computational methods have enabled previously intractable chemical problems to be solved using rigorous quantum-mechanical methods. This is the first comprehensive, up-to-date and technical work to cover all the important aspects of modern molecular electronic-structure theory. Topics covered in the book include:* Second quantization with spin adaptation* Gaussian basis sets and molecular-integral evaluation* H