1. Record Nr. UNINA9910451080103321

Autore	Schepel Harm
Titolo	The constitution of private governance : product standards in the regulation of integrating markets / / Harm Schepel
Pubbl/distr/stampa	Oxford ; ; Portland, Oregon : , : Hart Publishing, , 2005
ISBN	1-4725-6325-5 1-280-80847-0 9786610808472 1-84731-107-5
Edizione	[1st ed.]
Descrizione fisica	1 online resource (498 p.)
Collana	International studies in the theory of private law ; ; 4
Disciplina	343.087
Soggetti	Customary law Globalization Product safety - Law and legislation Product safety - Standards Electronic books.
Lingua di pubblicazione	Inglese
Formato	Materiale a stampa
Livello bibliografico	Monografia
Note generali	Originally presented as the author's thesis.
Nota di bibliografia	Includes bibliographical references (pages [415]-449) and index.
Nota di contenuto	Introduction -- 1 The Rise of Private Governance: Functional Differentiation and Economic Globalisation -- 2 The European Community: Market Integration and Private Transnationalism -- 3 The United States: Deregulation and Legalisation -- 4 Standards in the European Union -- 5 Standards and Codes in the United States -- 6 International Harmonisation of Standards -- 7 Private Regulation in European Public Law -- 8 Private Regulation in American Public Law -- 9 Politics and the Economy: Linking Institutions in Competition Law -- 10 Custom, Science and Law: Linking Institutions in Tort -- Conclusion The Constitution of Private Governance
Sommario/riassunto	In quantity and importance, private standards are rapidly taking over the role of public norms in the international and national regulation of product safety. This book provides a comprehensive overview of the rise, role and status of these private product safety standards in the legal regulation of integrating markets. In international and regional trade law as in European and American constitutional and

	administrative law, tort law and antitrust law, the book analyses the ways in which legal systems can and do recognise private norms as 'law.' This sociological question of law's recognition of private governance is indissolubly connected with a normative question of democratic theory: can law recognize legal validity and democratic legitimacy outside the constitution, without constitutional political institutions and beyond the nation state? Or: can law 'constitute' private transnational governance? The book offers the first systematic treatment of European, American and international 'standards law' in the English language, and makes a significant contribution to the study of the processes of globalization and privatization in social and legal theory. For the thesis on which this book was based Harm Schepel was awarded the first EUI Alumni Prize for the "best interdisciplinary and/or comparative thesis on European issues" written at the EUI in recent years

2.

Record Nr.	UNINA9910822436203321
Autore	Sholl David S
Titolo	Density functional theory : a practical introduction / / David S. Sholl and Jan Steckel
Pubbl/distr/stampa	Hoboken, N.J., : Wiley, c2009
ISBN	1-118-21104-9 1-282-13728-X 9786612137280 0-470-44771-0 0-470-44770-2
Edizione	[1st ed.]
Descrizione fisica	1 online resource (252 p.)
Classificazione	UL 2000 VE 5650
Altri autori (Persone)	SteckelJanice A
Disciplina	530.14/4
Soggetti	Density functionals Mathematical physics Quantum chemistry
Lingua di pubblicazione	Inglese
Formato	Materiale a stampa
Livello bibliografico	Monografia
Note generali	Includes index.

Nota di contenuto

DENSITY FUNCTIONAL THEORY; CONTENTS; Preface; 1 What Is Density Functional Theory?; 1.1 How to Approach This Book; 1.2 Examples of DFT in Action; 1.2.1 Ammonia Synthesis by Heterogeneous Catalysis; 1.2.2 Embrittlement of Metals by Trace Impurities; 1.2.3 Materials Properties for Modeling Planetary Formation; 1.3 The Schrodinger Equation; 1.4 Density Functional Theory-From Wave Functions to Electron Density; 1.5 Exchange-Correlation Functional; 1.6 The Quantum Chemistry Tourist; 1.6.1 Localized and Spatially Extended Functions; 1.6.2 Wave-Function-Based Methods; 1.6.3 Hartree-Fock Method
1.6.4 Beyond Hartree-Fock1.7 What Can DFT Not Do?; 1.8 Density Functional Theory in Other Fields; 1.9 How to Approach This Book (Revisited); References; Further Reading; 2 DFT Calculations for Simple Solids; 2.1 Periodic Structures, Supercells, and Lattice Parameters; 2.2 Face-Centered Cubic Materials; 2.3 Hexagonal Close-Packed Materials; 2.4 Crystal Structure Prediction; 2.5 Phase Transformations; Exercises; Further Reading; Appendix Calculation Details; 3 Nuts and Bolts of DFT Calculations; 3.1 Reciprocal Space and k Points; 3.1.1 Plane Waves and the Brillouin Zone
3.1.2 Integrals in k Space3.1.3 Choosing k Points in the Brillouin Zone; 3.1.4 Metals-Special Cases in k Space; 3.1.5 Summary of k Space; 3.2 Energy Cutoffs; 3.2.1 Pseudopotentials; 3.3 Numerical Optimization; 3.3.1 Optimization in One Dimension; 3.3.2 Optimization in More than One Dimension; 3.3.3 What Do I Really Need to Know about Optimization?; 3.4 DFT Total Energies-An Iterative Optimization Problem; 3.5 Geometry Optimization; 3.5.1 Internal Degrees of Freedom; 3.5.2 Geometry Optimization with Constrained Atoms; 3.5.3 Optimizing Supercell Volume and Shape; Exercises; References Further ReadingAppendix Calculation Details; 4 DFT Calculations for Surfaces of Solids; 4.1 Importance of Surfaces; 4.2 Periodic Boundary Conditions and Slab Models; 4.3 Choosing k Points for Surface Calculations; 4.4 Classification of Surfaces by Miller Indices; 4.5 Surface Relaxation; 4.6 Calculation of Surface Energies; 4.7 Symmetric and Asymmetric Slab Models; 4.8 Surface Reconstruction; 4.9 Adsorbates on Surfaces; 4.9.1 Accuracy of Adsorption Energies; 4.10 Effects of Surface Coverage; Exercises; References; Further Reading; Appendix Calculation Details
5 DFT Calculations of Vibrational Frequencies5.1 Isolated Molecules; 5.2 Vibrations of a Collection of Atoms; 5.3 Molecules on Surfaces; 5.4 Zero-Point Energies; 5.5 Phonons and Delocalized Modes; Exercises; Reference; Further Reading; Appendix Calculation Details; 6 Calculating Rates of Chemical Processes Using Transition State Theory; 6.1 One-Dimensional Example; 6.2 Multidimensional Transition State Theory; 6.3 Finding Transition States; 6.3.1 Elastic Band Method; 6.3.2 Nudged Elastic Band Method; 6.3.3 Initializing NEB Calculations; 6.4 Finding the Right Transition States
6.5 Connecting Individual Rates to Overall Dynamics

Sommario/riassunto

Demonstrates how anyone in math, science, and engineering can master DFT calculations Density functional theory (DFT) is one of the most frequently used computational tools for studying and predicting the properties of isolated molecules, bulk solids, and material interfaces, including surfaces. Although the theoretical underpinnings of DFT are quite complicated, this book demonstrates that the basic concepts underlying the calculations are simple enough to be understood by anyone with a background in chemistry, physics, engineering, or mathematics. The authors show how the widespread