

1. Record Nr.	UNINA9910830664003321
Autore	Alavi Saman
Titolo	Molecular simulations : fundamentals and practice / / Saman Alavi
Pubbl/distr/stampa	Weinheim, : Wiley-VCH, c2020 Weinheim, Germany : , : Wiley-VCH, , [2020] ©2020
ISBN	3-527-69946-5 3-527-69953-8 3-527-69945-7
Descrizione fisica	1 online resource (345 pages)
Classificazione	431.1 541.22
Disciplina	541.22
Soggetti	Molecular structure
Lingua di pubblicazione	Non definito
Formato	Materiale a stampa
Livello bibliografico	Monografia
Note generali	Includes bibliographical references (p. 297-315) and index
Nota di contenuto	Front Matter -- Introduction -- Studying Systems from Two Viewpoints -- Classical Mechanics and Numerical Methods -- Intra- and Intermolecular Potentials in Simulations -- The Mechanics of Molecular Dynamics -- Probability Theory and Molecular Simulations -- Statistical Mechanics in Molecular Simulations -- Thermostats and Barostats -- Simulations of Structural and Thermodynamic Properties -- Simulations of Dynamic Properties -- Monte Carlo Simulations.
Sommario/riassunto	Provides hands-on knowledge enabling students of and researchers in chemistry, biology, and engineering to perform molecular simulations This book introduces the fundamentals of molecular simulations for a broad, practice-oriented audience and presents a thorough overview of the underlying concepts. It covers classical mechanics for many-molecule systems as well as force-field models in classical molecular dynamics; introduces probability concepts and statistical mechanics; and analyzes numerous simulation methods, techniques, and applications. Molecular Simulations: Fundamentals and Practice starts by covering Newton's equations, which form the basis of classical mechanics, then continues on to force-field methods for modelling potential energy surfaces. It gives an account of probability concepts

before subsequently introducing readers to statistical and quantum mechanics. In addition to Monte-Carlo methods, which are based on random sampling, the core of the book covers molecular dynamics simulations in detail and shows how to derive critical physical parameters. It finishes by presenting advanced techniques, and gives invaluable advice on how to set up simulations for a diverse range of applications. -Addresses the current need of students of and researchers in chemistry, biology, and engineering to understand and perform their own molecular simulations -Covers the nitty-gritty ' from Newton's equations and classical mechanics over force-field methods, potential energy surfaces, and probability concepts to statistical and quantum mechanics -Introduces physical, chemical, and mathematical background knowledge in direct relation with simulation practice - Highlights deterministic approaches and random sampling (eg: molecular dynamics versus Monte-Carlo methods) -Contains advanced techniques and practical advice for setting up different simulations to prepare readers entering this exciting field

**Molecular Simulations: Fundamentals and Practice** is an excellent book benefitting chemist, biologists, engineers as well as materials scientists and those involved in biotechnology.

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2. Record Nr.	UNINA9910971136903321
Titolo	Right-wing extremism in the twenty-first century // editors, Peter H. Merkl, Leonard Weinberg
Pubbl/distr/stampa	London ; ; Portland, Or., : Frank Cass, 2003
ISBN	1-135-76420-4 0-7146-5182-6 1-135-76421-2 1-280-10382-5 0-203-49791-0
Edizione	[2nd rev. ed.]
Descrizione fisica	xv, 311 p
Collana	Cass series on political violence
Altri autori (Persone)	MerklPeter H WeinbergLeonard <1939->
Disciplina	320.53/09/05
Soggetti	Right-wing extremists Radicalism
Lingua di pubblicazione	Inglese
Formato	Materiale a stampa
Livello bibliografico	Monografia
Note generali	Rev. ed. of: The revival of right-wing extremism in the nineties.
Nota di bibliografia	Includes bibliographical references and index.
Nota di contenuto	chapter Introduction -- part Part 1 The Extreme Right in the Ascendancy -- chapter 1 Stronger than Ever -- chapter 12 Theories of the Extreme Right -- chapter 3 The Growing Threat of the Radical Right / Hans-Georg Betz -- part Part 2 Comparing Public Opinion Indicators -- chapter 4 Racism and the Political Right: European Perspectives -- chapter 5 Explaining National Variations in Support for Far Right Political Parties in Western Europe, 1990-2000 / Allen Wilcox -- chapter 6 The Development of the Extreme Right at the End of the Century / Piero Ignazi -- part Part 3 Changing National Contexts -- chapter 7 The Front National in Context: French and European Dimensions -- chapter 8 The FP: From Populist Protest to Incumbency / Kurt Richard Luther -- chapter 9 Right-Wing Extremism and Xenophobia in Germany: Escalation, Exaggeration, or What? / Ekkart Zimmermann -- chapter 10 Right-Wing Extremism in Russia: The Dynamics of the 1990s / Vera Tolz -- chapter 11 Patterns of Response to the Extreme Right in Western Europe.
Sommario/riassunto	Revising the 1997 first edition, this study covers events that occurred

in Oldham and Bradford after the year 2000.

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