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Titolo	Information Science for Materials Discovery and Design / / edited by Turab Lookman, Francis J. Alexander, Krishna Rajan
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Edizione	[1st ed. 2016.]
Descrizione fisica	1 online resource (316 p.)
Collana	Springer Series in Materials Science, , 0933-033X ; ; 225
Disciplina	620.11
Soggetti	Nanotechnology Engineering—Materials Data mining Statistical physics Dynamical systems Materials science Materials Engineering Data Mining and Knowledge Discovery Complex Systems Characterization and Evaluation of Materials Statistical Physics and Dynamical Systems
Lingua di pubblicazione	Inglese
Formato	Materiale a stampa
Livello bibliografico	Monografia
Note generali	Description based upon print version of record.
Nota di bibliografia	Includes bibliographical references at the end of each chapters and index.
Nota di contenuto	From the Contents: Introduction -- Data-Driven Discovery of Physical, Chemical, and Pharmaceutical Materials -- Cross-Validation and Inference in Bioinformatics/Cancer Genomics -- Applying MQSPRs - New Challenges and Opportunities.
Sommario/riassunto	This book deals with an information-driven approach to plan materials discovery and design, iterative learning. The authors present contrasting but complementary approaches, such as those based on high throughput calculations, combinatorial experiments or data driven discovery, together with machine-learning methods. Similarly, statistical methods successfully applied in other fields, such as biosciences, are presented. The content spans from materials science

to information science to reflect the cross-disciplinary nature of the field. A perspective is presented that offers a paradigm (codesign loop for materials design) to involve iteratively learning from experiments and calculations to develop materials with optimum properties. Such a loop requires the elements of incorporating domain materials knowledge, a database of descriptors (the genes), a surrogate or statistical model developed to predict a given property with uncertainties, performing adaptive experimental design to guide the next experiment or calculation and aspects of high throughput calculations as well as experiments. The book is about manufacturing with the aim to halving the time to discover and design new materials. Accelerating discovery relies on using large databases, computation, and mathematics in the material sciences in a manner similar to the way used to in the Human Genome Initiative. Novel approaches are therefore called to explore the enormous phase space presented by complex materials and processes. To achieve the desired performance gains, a predictive capability is needed to guide experiments and computations in the most fruitful directions by reducing not successful trials. Despite advances in computation and experimental techniques, generating vast arrays of data; without a clear way of linkage to models, the full value of data driven discovery cannot be realized. Hence, along with experimental, theoretical and computational materials science, we need to add a “fourth leg’’ to our toolkit to make the “Materials Genome'' a reality, the science of Materials Informatics.