Computational Methods For Predicting Material Processing Defects

#material defect prediction #computational modeling defects #processing defect simulation #manufacturing quality control #materials science predictive analytics

Explore advanced computational methods for accurately predicting material processing defects. Enhance manufacturing quality and reduce failures through predictive modeling and simulation techniques.

Computational Methods For Predicting Material Processing Defects

Balling defect prediction in additive manufacturing using machine learning - Balling defect prediction in additive manufacturing using machine learning by Additive Manufacturing and Welding 890 views 2 years ago 12 minutes, 30 seconds - Producing **defect**,-free, high-quality additive manufacturing parts in a time-efficient and cost-effective way is a major challenge to ...
Physics-informed machine learning and mechanistic modeling of additive manufacturing to reduce defects
Balling defect in additive manufacturing
Main objectives
Road map of this work
Effect of the six mechanistic variables on balling
3D temperature and velocity distributions calculation
Balling Susceptibility Index (BSI) to predict balling in PBF-L
Relative importance of the six mechanistic variables
Hierarchical influence of six mechanistic variables on balling
Distribution of two most important mechanistic variables
Process maps and BSI values for six alloys
Conclusions
Tutorial: Understanding and Computational Modelling of Defects in Semiconductors (with VASP) - Tutorial: Understanding and Computational Modelling of Defects in Semiconductors (with VASP) by Seán R. Kavanagh 10,309 views 2 years ago 1 hour, 39 minutes - Tutorial talk on understanding and computationally modelling **defects**, in semiconductors (using plane wave DFT with VASP).
Tutorial: Modelling Point Defects in Semiconductors with VASP (Audio Fix) - Tutorial: Modelling Point Defects in Semiconductors with VASP (Audio Fix) by Seán R. Kavanagh 5,453 views 1 year ago 2 hours, 11 minutes - **Now with bonus 25 minutes intro to **defect**, structure searching and

ShakeNBreak** Tutorial talk on understanding and ...
Importance of Defects
Intrinsic versus Extrinsic
Examples
Chemical Potential
Thermodynamic Definition
Zinc Oxide
Calculate the Chemical Potential Limits of Titanium
Defect Formation Energy Diagrams
Shallow Defect
Chemical Potentials
Configurational Entropy
Defect Formation Energy Diagram
Self-Consistent Fermi Level
Material Properties
Optical Behavior
Configuration Coordinate Diagram
Transition Level Diagram
Dlts
Intro
Introduction
Alternative Structure Searching Approaches
Evolutionary Algorithm Approach
Summary
Overview
The Workflow
Extrinsic Substitutions
Setting Different Charge Dates for Defects
Correction Schemes
Takeaways
Relaxation Pre-Convergence
Input Files
Charge Correction Plots
Sample Input File
Tetrahedron Smearing
Defect Transition Level Diagram
Structure Visualization
Computational and predictive methods for risk assessment : issues and promises - Computational and predictive methods for risk assessment : issues and promises by Anses - Agence nationale de sécurité sanitaire 268 views 3 years ago 2 hours, 19 minutes - David Demortain (LISIS), chairman , Frédéric Bois (CERTARA), Kathryn Guyton (IARC), Jean-Lou Dorne (EFSA), Anax Oliveira ...
Introduction
Safety Factors
Computational Toxicology
Conditional Toxicity Value Predictor
How Do You Select and Prioritize Uh Agents for Assessment
Importance of Public Availability
Challenges
How Do You Avoid Bias towards a Favored Mechanism
Viruses
Inducing Oxidative Stress
Scope of Activity
Transparency in Risk Assessment
Hazard Identification
Exposure Assessment
Weight of Evidence
Concluding Thoughts
User Guide
Differences between Countries and Regulatory Frameworks

The Question of Systems Biology
Reproducibility
Internal Quality Assurance
Issues with Robustness and Assessment of Complex Models
How Artificial Intelligence Models Work
The Expert Rule-Based System
Expert Review
Validation of Pvpk Models
Apra Accelerating the Pace of Chemical Risk Assessment
Computational discovery of 2D materials - Computational discovery of 2D materials by Advanced Materials Congress Lectures 88 views 1 year ago 23 minutes - Full Title: **Computational**, discovery of 2D **materials**,: a fundament study of boron sheets and phosphide binary compounds ...
Computational modeling for materials discovery
Unique Properties of Low-Dimensional Mat
Functional Design for Vast Range of Applicati
Routes of Computational Discovery (Cont.)
Predictions of Low Dimensional Materials
Two-Dimensional Boron Sheets Based on Icosahe
Prediction of 2D Icosahedral B•, Structures
Structural Stabilization of 2D Icosahedral B
Energetics and Band Gaps of 2D Icosahedral
Energy Barriers of 2D Icosahedral B•,
Prediction of 2D GaP/InP Binary Compound
Discovery of 2D Sandwiched GaP/InP Binary Comp
Energetics and Structural Properties
Our Ongoing Researches
A Possible Pathway to Synthesize Blue Phosphore
Acknowledgement
Materials by Design | Enhancing materials and formulations with computational modelling - Materials by Design | Enhancing materials and formulations with computational modelling by Science and Technology Facilities Council 297 views 8 months ago 2 minutes, 41 seconds - How can **computational**, modelling at the atomic scale enable industry to create more effective **materials**, products and formulations ...
Advances in Methods and Applications in Computational Chemistry and Materials Science - Advances in Methods and Applications in Computational Chemistry and Materials Science by PASC Conference 271 views 1 year ago 1 minute, 42 seconds - Introduction of the Minisymposium "Advances in **Methods**, and Applications in **Computational**, Chemistry and **Materials**, Science", ...
Introduction
Speakers
Theme
Computational techniques to predict crack growth in nonlinear viscoelastic materials - Computational techniques to predict crack growth in nonlinear viscoelastic materials by European Structural Integrity Society 81 views 7 years ago 16 minutes - Isaac India in modeling cracks and then i will look at the applications of these **methods**, in first for cracking and then a d1 all ...
All Machine Learning Models Explained in 5 Minutes | Types of ML Models Basics - All Machine Learning Models Explained in 5 Minutes | Types of ML Models Basics by Learn with Whiteboard 1,119,160 views 3 years ago 5 minutes, 1 second - Confused about understanding machine learning models? Well, this video will help you grab the basics of each one of them.
Introduction
Overview
Supervised Learning
Linear Regression
Decision Tree
Random Forest
Neural Network
Classification
Support Vector Machine
Classifier
Unsupervised Learning

Dimensionality Reduction
Talk to the spirits of the deceased || Spiritual Response Mantra - Talk to the spirits of the deceased || Spiritual Response Mantra by Th§n Chú Linh èng 845 views 2 days ago 2 hours, 6 minutes - In this YouTube video, stories are told about how to talk to spirits, how to summon the spirits of the deceased, and how ...
Recyclable Waste Classifier using Opencv Python | Computer Vision - Recyclable Waste Classifier using Opencv Python | Computer Vision by Murtaza's Workshop - Robotics and AI 37,711 views 1 year ago 56 minutes - #ComputerVision #OpenCV #CVZone.
What is dark matter? – with Peter Fisher - What is dark matter? – with Peter Fisher by The Royal Institution 237,198 views 1 year ago 56 minutes - What exactly is dark matter? We can't see it, but we can observe its ghostly gravitational effects on the behaviour and evolution of ...
Introduction
History of particle physics
Outline
Expanding Universe
Hubble Extremely Deep Field
Examples of Dark Matter
The Coma Cluster
The Schmidt Telescope
Andromeda
Standard Model
Galaxy
Particles
Double beta Decay
CDMS
Axions
87 Getting Your Data Ready Convert Data To Numbers | Scikit-learn Creating Machine Learning Models - 87 Getting Your Data Ready Convert Data To Numbers | Scikit-learn Creating Machine Learning Models by Machine Learning 19,368 views 2 years ago 16 minutes - ... ensemble import random forest regressor and if you remember back in our workflow we were **predicting**, a classification problem ...
How Robots Grow and Harvest Millions of Vegetables Every Day - How Robots Grow and Harvest Millions of Vegetables Every Day by Farm Front 46,158 views 6 days ago 29 minutes - How Robots Grow and Harvest Millions of Vegetables Every Day Discover the future of agriculture in our video, "How Robots ...
Miller indices simplest explaination| animation - Miller indices simplest explaination| animation by Telutron 224,554 views 2 years ago 5 minutes, 13 seconds - Miller Indices ,lattice plane ,and problems explained Accredition: ...
Machine Learning Tutorial Python - 7: Training and Testing Data - Machine Learning Tutorial Python - 7: Training and Testing Data by codebasics 458,790 views 5 years ago 6 minutes, 34 seconds - sklearn.model_selection.train_test_split **method**, is used in machine learning projects to split available dataset into training and ...
Theory behind why we need to split given dataset into training and test using sklearn train set split method.
Coding (Here we use car price prediction problem to demonstrate train test split)
Use train_test_split from sklearn
Use of random state method
Use of fit() method to train your model
Score() method (to check the accuracy of the model)
Simulated Annealing - Simulated Annealing by Adam Gaweda 7,644 views 1 year ago 17 minutes - ... blacksmith we're in a forge you know we're heating up and banging the swords and what's happening as that whole **process**, is ...
AI vs Machine Learning - AI vs Machine Learning by IBM Technology 812,872 views 11 months ago 5 minutes, 49 seconds - What is really the difference between Artificial intelligence (AI) and machine learning (ML)? Are they actually the same thing?
Computer modelling for molecular science – with Sir Richard Catlow - Computer modelling for molecular science – with Sir Richard Catlow by The Royal Institution 24,311 views 1 year ago 1 hour - High-performance, realistic **computer**, simulations are crucially important for science and engineering, even allowing scientists **to**, ...

Modelling molecules and materials
Using modelling for crystallography
Genetic algorithms for predicting crystal structures
Lawrence Bragg and the bubble raft
High performance computer modelling of materials
Modelling of nanostructures and nanoparticles
High energy density batteries
Three challenges for modelling
95 Making Predictions With Our Model | Scikit-learn Creating Machine Learning Models - 95 Making Predictions With Our Model | Scikit-learn Creating Machine Learning Models by Machine Learning 33,904 views 2 years ago 8 minutes, 25 seconds - ... we're finally going to use a trained machine learning model to make some **predictions**, right this is where the magic and machine ...
Machine Learning Based Predictive Quality - Machine Learning Based Predictive Quality by PSI Metals 118 views 1 year ago 13 minutes, 56 seconds - In steel production, machine learning models explore all possible combinations of how production factors affect quality metrics ...
Advances in first-principles computational materials science - Advances in first-principles computational materials science by NanoBio Node 8,279 views 11 years ago 55 minutes - Advances in first-principles **computational materials**, science Dr. Elif Ertekin, Mechanical Science & Engineering, University of ...
Materials Challenges
Automobile Waste Heat Recovery Systems
Hydrogen Powered Bus
Integrated Circuits
The Schrodinger Equation
Schrodinger Equation
Density Functional Theory
Notes on on Density Functional Theory
Design for Photocatalysis
High Accuracy Modeling of Defects in Semiconductors Using Quantum Monte Carlo Methods
Particle Balancing Equation
Optical Ionisation
Optical Ionization Energy
Charge Distributions
Defect Formation Energies
Quantum Monte Carlo
Quantum Monte Carlo Code
Optical Transition Energies
Zinc Oxide
Bridging computational and experimental predictions in materials machine learning models - Bridging computational and experimental predictions in materials machine learning models by Materials Virtual Lab 587 views 2 years ago 30 minutes - Prof Ong gave a talk on bridging **computational**, and experimental **predictions**, in **materials**, machine learning models at the CNLS ...
Intro
Graph deep learning models
Bayesian Optimization with Symmetry Relaxation of Structures
Learning from multi-fidelity data
Machine learning interatomic potentials
ML-IAP studies of lithium superionic conductors
Conclusions
Julia Ling: "Machine Learning for Materials Discovery" | IACS Seminar - Julia Ling: "Machine Learning for Materials Discovery" | IACS Seminar by Harvard Institute for Applied Computational Science 13,999 views 5 years ago 50 minutes - Presented by Dr. Julia Ling, Director of Data Science at Citrine Informatics Talk abstract: **Materials**, science presents a unique set ...
Introduction
Julia Ling
Why do we need machine learning
Why is this hard
Data types
Microstructure

Model Accuracy
Data Volume
Transfer Learning
Domain Knowledge
Band Gap in Color
Interpretability
Example
Uncertainty quantification
Sequential learning
Results
Ongoing research
Training data coverage
Key takeaways
Questions
James Kermode - Multiscale and data-driven methods for the simulation of material failure - James Kermode - Multiscale and data-driven methods for the simulation of material failure by Institute for Pure & Applied Mathematics (IPAM) 233 views 11 months ago 53 minutes - Recorded 19 April 2023. James Kermode of the University of Warwick presents "Multiscale and data-driven **methods**, for the ...
Intro
Motivation: Chemomechanical Processes
Atomistic Modelling of Brittle Fracture
Fracture toughness of silicon carbide - 6H & 3C polymorphs
Concurrent Multiscale Materials Modelling
QM Region Selection
Constrained retraining for QM/ML embedding
Energetics of fracture- continuum
Lattice trapping barriers to brittle fracture
Coupling to Continuum BCs for Fracture of Amorphous Carbon
NCFlex: flexible boundary conditions + numerical continuation
SOAP/GAP Machine Learning Interatomic Potentials
Large datasets: parallelisation of GAP fitting code
GAP predictive variance - vacancy migration
Calibrating Uncertainties with Conformal Prediction
Application to silicon: elastic constants
Learning Hamiltonians from DFT data
Prediction accuracy for Hamiltonian and overlap
Systematic convergence of electronic structure
Generalisability and transferability
ACE Hamiltonian Model for Silicon
FEM@LLNL | Fast, Accurate and Large-scale Ab-initio Calculations for Materials Modeling - FEM@LLNL | Fast, Accurate and Large-scale Ab-initio Calculations for Materials Modeling by Livermore Lab Events 457 views 10 months ago 1 hour, 12 minutes - Sponsored by the MFEM project, the FEM@LLNL Seminar Series focuses on finite element research and applications talks of ...
Seminar: Predicting the Atomic Structures of Defects - Seminar: Predicting the Atomic Structures of Defects by Seán R. Kavanagh 245 views 5 months ago 36 minutes - Abstract: **Defects**, are a universal, unavoidable feature of solid **materials**,, controlling properties and performance in most functional ...
Microstructure prediction through multiscale modeling of solidification processing by Damien Tourret - Microstructure prediction through multiscale modeling of solidification processing by Damien Tourret by IMDEA Materials Institute 2,503 views 3 years ago 1 hour, 4 minutes - Topics covered during the webinar: - Fundamentals of microstructure formation in solidification **processing**, (e.g. casting, welding, ...
Outline
Casting of Metallic Alloys
Microstructure matters
Multiscale modeling @ IMDEA Materials
Multiscale modeling of solidification

Grain boundaries
Mechanisms of GB selection
Three-dimensions: effect of azimuthal angle B
Multiscale Cellular Automaton approach
Upscaling from phase-field results
Complex multicomponent alloys
Cell / Dendrite scale
Grain structure scale
Process scale
Selective Laser Melting of Inconel 718
Alloy / Process variability
Object Detection Explained | Tensorflow Object Detection | AI ML for Beginners | Edureka - Object Detection Explained | Tensorflow Object Detection | AI ML for Beginners | Edureka by edureka! 59,401 views 3 years ago 2 minutes, 35 seconds - #PythonEdureka #Edureka #objectdetection #pythonprojects #pythonprogramming #pythontutorial #PythonTraining ...
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