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Computer Modeling in Inorganic Crystallography - 1st Edition

1.5.1 Atomistic Simulations. Atomistic simulations, the most widely used methods in the nanomechanics field, are important numerical methods for the investigation of magnetic, electronic, chemical, and mechanical properties of carbon nanostructures since these modeling approaches can accurately trace atomic position and precisely capture the microscale physical mechanism, such as buckling. There has been already much research of carbon nanostructures using atomistic simulation.

Atomistic Simulation - an overview | ScienceDirect Topics

Recent work using atomistic simulations on a number of different oxide and mineral interfaces is described. Static simulation techniques have been applied to gadolinium doped ceria grain boundaries and show that there is marked variation in oxygen vacancy and dopant segregation with depth and orientation of a number of tilt boundaries.

Atomistic modelling of adsorption and segregation at ...

An introduction to atomistic simulation methods 9 where θ_0 is the nominal equilibrium angle (90° for an octahedral coordination, 109.47° for a tetrahedral coordination). Other functions, such as more complicated distance-dependent pair terms, or multi-atom terms, can be incorporated into a model, provided

An Introduction to atomistic simulation methods

This course uses the theory and application of atomistic computer simulations to model, understand, and predict the properties of real materials. Specific topics include: energy models from classical potentials to first-principles approaches; density functional theory and the total-energy pseudopotential method; errors and accuracy of quantitative predictions: thermodynamic ensembles, Monte ...

Atomistic Computer Modeling of Materials (SMA 5107 ...

Atomistic computer simulations in chemistry: standard and advanced approaches Computational chemistry is the study of chemical systems by means of computer simulations. It comprises different types of approaches such as coarse-grained models, classical molecular dynamics, semi-empirical simulations and ab initio quantum chemistry methods (see ...

Prebiotic chemistry and origins of life research with ...

Using atomistic computer simulations we determine the roughness and topographical features of melt-formed (MS) and fracture surfaces (FS) of oxide glasses. We find that the topography of the MS is...

Fracture, Surface, and Structure of Silicate Glasses ...

1. J Nanosci Nanotechnol. 2009 May;9(5):2795-812. Atomistic simulations of inorganic nanowires. Dai L(1), Tan VB, Sow CH, Lim CT. Author information: (1)NUS Nanoscience and Nanotechnology Initiative, National University of Singapore S117576, Singapore Inorganic nanowires, such as those of metals, semiconductors and oxides, have attracted much research interest due to their unique material ...

Atomistic simulations of inorganic nanowires.

Object of study. Due to the intrinsic restrictions on the accessible time scales of all-atom Molecular Dynamics (MD) simulations, we aim in this study at revealing clustering tendencies—rather than a large scale self-assembly—of specific organic components in solution in the presence of inorganic components. We further aim at exploring the relevant physical interactions (electrostatic ...

Exploring the organic-inorganic interface in biosilica ...

The effect of inorganic filler on the thermal properties of a polyimide-SiO₂ nanocomposite was studied using atomistic molecular dynamics simulation. The increase in the weight content of the filler above a particular threshold (about 20%) was shown to cause a sharp drop in the temperature coefficient of the linear expansion of the material.

Effect of inorganic filler on the thermal properties of ...

Focus is placed on candidates with a demonstrated expertise in atomistic simulations. Open positions: The successful candidates will work on projects related to atomistic simulations of non-crystalline materials. Topics of interest include, but are not limited to: - Classical, reactive, and ab initio simulations of inorganic materials.

University Job: Postdoc in Atomistic Simulations of ...

Peng Shi, Hui Zhang, Lin Lin, Chunhui Song, Qingguo Chen, Zesheng Li. Molecular dynamics study of the effect of inorganic salts on the monolayer of four surfactants at the oil/water interface, Journal of Dispersion Science and Technology, 10.1080/01932691.2018.1462200, 39, 12, (1758-1766), (2018).

Effect of Na+ and Ca2+ ions on a Lipid Langmuir Monolayer ...

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Generalized continuum mechanics (GCM) has attracted increased attention in the context of multiscale materials modeling, an example of which is a bottom-up GCM model, called the atomistic field...

Generalized Continua Concepts In Coarse-Graining Atomistic ...

Lithium stannate (Li₂SnO₃) is currently being considered as a material for electrode and electrode coating applications in Li-ion batteries. The intrinsic defect formation and Li-ion transport properties of Li₂SnO₃ doped with divalent and trivalent transition-metal dopants (Mn, Fe, Co, and Ni) are explored in this work using atomistic simulations. Defect formation simulations reveal that all ...