Research outputs
Listing of Research outputs

Local volume effects in the generalized pseudopotential theory
Research output: Contribution to journal › Article

Embrittlement of an elasto-plastic medium by an inclusion
Research output: Contribution to journal › Article

Effects of calcium on planar fault energies in ternary magnesium alloys
Research output: Contribution to journal › Article

Density functional theory calculations of iron - vanadium carbide interfaces and the effect of hydrogen
Research output: Contribution to journal › Article

A Crystal Plasticity Assessment of Normally-loaded Sliding Contact in Rough Surfaces and Galling
Research output: Contribution to journal › Article

Hydrogen diffusion and trapping in alpha-iron: The role of quantum and anharmonic fluctuations
Research output: Contribution to journal › Letter

Hydrogen embrittlement II. Analysis of hydrogen-enhanced decohesion across (111) planes in α-Fe
Research output: Contribution to journal › Article

Hydrogen embrittlement I. Analysis of hydrogen-enhanced localized plasticity: Effect of hydrogen on the velocity of screw dislocations in α-Fe
Research output: Contribution to journal › Article

Theoretical evaluation of the role of crystal defects on local equilibrium and effective diffusivity of hydrogen in iron
Research output: Contribution to journal › Article

The challenges of hydrogen and metals
Research output: Chapter in Book/Report/Conference proceeding › Conference paper

Quantum and isotope effects on hydrogen diffusion, trapping and escape in iron
Research output: Contribution to journal › Article

Universal tight binding model for chemical reactions in solution and at surfaces. I. Organic molecules
Research output: Contribution to journal › Article
Universal tight binding model for chemical reactions in solution and at surfaces. III. Stoichiometric and reduced surfaces of titania and the adsorption of water
Research output: Contribution to journal › Article

From quantum mechanics to physical metallurgy of steels
Research output: Contribution to journal › Article

Industrially-Relevant Multiscale Modelling of Hydrogen Assisted Degradation
Research output: Chapter in Book/Report/Conference proceeding › Conference paper

Quantum rate theory of the trapping of hydrogen and deuterium by a vacancy in iron
Research output: Chapter in Book/Report/Conference proceeding › Conference paper

Universal tight binding model for chemical reactions in solution and at surfaces. II. Water
Research output: Contribution to journal › Article

Fully quantum mechanical calculation of the diffusivity of hydrogen in iron using the tight-binding approximation and path integral theory
Research output: Contribution to journal › Article

Analysis of a carbon dimer bound to a vacancy in iron using density functional theory and a tight binding model
Research output: Contribution to journal › Article

Practical applications of first principles and empirical quantum mechanics in materials modelling
Research output: Chapter in Book/Report/Conference proceeding › Conference paper

An ignition key for atomic-scale engines
Research output: Contribution to journal › Article

Is the pinning of ordinary dislocations in γ-TiAl intrinsic or extrinsic in nature? A combined atomistic and kinetic Monte Carlo approach
Research output: Contribution to journal › Article

A tight binding model for water
Research output: Contribution to journal › Article
MultiHy: an EU-FP7-NMP Project on Multiscale Modelling of Hydrogen Embrittlement
Research output: Chapter in Book/Report/Conference proceeding › Conference paper

Nonconservative current-induced forces: A physical interpretation
Research output: Contribution to journal › Article

Microscopic origin of channeled flow in lamellar titanium aluminide
Research output: Contribution to journal › Article

Electronic structure and total energy of interstitial hydrogen in iron: Tight-binding models
Research output: Contribution to journal › Article

Ring currents in azulene
Research output: Contribution to journal › Article

Atomistic studies of interactions between the dominant lattice dislocations and γ/γ-lamellar boundaries in lamellar γ-TiAl
Research output: Contribution to journal › Article

Boron in copper: A perfect misfit in the bulk and cohesion enhancer at a grain boundary
Research output: Contribution to journal › Article

Magnetic tight binding and the iron-chromium enthalpy anomaly
Research output: Contribution to journal › Article

Atomistic study of ordinary 1/2 〈110〉 screw dislocation core structures and glide in γ-TiAl
Research output: Contribution to journal › Article

Structural and chemical embrittlement of grain boundaries by impurities: A general theory and first-principles calculations for copper
Research output: Contribution to journal › Article

Theory of the near K-edge structure in electron energy loss spectroscopy
Research output: Contribution to journal › Article
Effect of relaxation on the oxygen K-edge electron energy-loss near-edge structure in yttria-stabilized zirconia

Relative energetics and structural properties of zirconia using a self-consistent tight-binding model

The near-edge structure in energy-loss spectroscopy: many-electron and magnetic effects in transition metal nitrides and carbides

Effect of material properties on stress-induced defect generation in trenched SOI

Comment on "Origin of the modulated phase in copper-gold alloys" - Reply

Crystal structures of zirconia from first principles and self-consistent tight binding

Electronic structure of 5d transition metals adsorbed on the stoichiometric (110) rutile surface

Stabilizing role of itinerant ferromagnetism in intergranular cohesion in iron

The role of planar fault energy in the yield anomaly in L1(2) intermetallics

Electronic structure of reduced titanium dioxide

Self-consistent tight-binding approximation including polarisable ions
Structural stability of NiTi2 intermetallic compounds
Research output: Contribution to journal › Article

Al3Ru-A ductile trialuminide?
Research output: Contribution to journal › Article

First-principles determination of the Ni-Al phase diagram
Research output: Contribution to journal › Article

A quantum-mechanical calculation of the theoretical strength of metals
Research output: Contribution to journal › Article

RECENT ADVANCES IN NON SELF-CONSISTENT TOTAL ENERGY CALCULATIONS IN ALLOYS
Research output: Chapter in Book/Report/Conference proceeding › Conference paper

A tight-binding study of grain boundaries in silicon
Research output: Contribution to journal › Article

High-precision sampling for Brillouin-zone integration in metals
Research output: Contribution to journal › Article

INTERATOMIC FORCES AND BOND-ENERGIES IN THE TIGHT-BINDING APPROXIMATION
Research output: Chapter in Book/Report/Conference proceeding › Conference paper

INTERATOMIC FORCES IN TRANSITION-METALS
Research output: Contribution to journal › Article