

Company Overview



Outline

- Company profile
- Technology positioning
- Customers and products
- The MedeA software platform

Company Profile

- Materials Design, Inc. started in 1998 in San Diego, California, USA
- 1999: Creation of European branch in France
- Core competence:
 - computational chemistry, physics, and materials science
 - materials property databases
 - scientific software engineering
- Global network of technology partners including:
 - University of Vienna VASP
 - University of Cracow Phonon
 - Pierre Villars Pauling File, structural databases and phase diagrams
 - FIZ Karlsruhe ICSD, ASM Intl. Pearson's crystal data, NIST
 - IFP and University of Paris GIBBS
 - Sandia National Laboratory LAMMPS
 - J. J. P. Stewart MOPAC
- Business partners
 - Japan: Ryoka Systems
 - China: Beijing Hongcam Software
 - India: Apsara Innovations

Technology Positioning



Products and Services

Licensing and support of MedeA software

- Includes training, online support, and maintenance
- Annual users group meetings

Contract research

- Solution of specific problems
- Leverages expertise and resources of MD's scientists
- Technology partnerships
 - Development of customized modeling capabilities



Global Presence



Customers

Industry

- Automotive
- Energy and power generation
- Aerospace
- Chemical and petrochemical
- Steel and metal alloys
- Electronics
- Glass and ceramics
- Display and lighting
- Drilling and mining
- Government research laboratories
- Universities

Some Commercial Customers



Some Government and Not-For Profit Customers













Routh Aparts Press (abstrate)











Rationale for MedeA Software



Purpose of MedeA

Understand and predict any physical and chemical property of any combination of materials



Approaches:

- Ab initio electronic structure calculations
- Forcefield simulations
- Statistical mechanics
- Analytical theory
- Empirical correlations
- Experimental data of existing materials (databases) as reference

Computed Materials Properties

Structural properties

- Molecular structures
- Crystal structures
- Surface structures
- Structure around defects
- Adsorption geometries
- Structures of interfaces
- Liquids and amorphous systems

Thermo-Mechanical properties

- Elastic moduli
- Speed of sound
- Vibrational properties
- Thermal expansion coefficients
- Fracture

Thermodynamic properties

- ΔU , ΔH , ΔS , ΔG , heat capacity,
- Binding energies
- Solubility
- Melting temperature
- Vapor pressure
- Miscibility
- Phase diagrams
- Surface tension

Chemical properties

- Chemical reaction rates in gases and condensed phases
- Reactivity on surfaces
- Solid-solid reactions
- Pressure-induced reactions
- Photochemical reactions

Transport properties

- Mass diffusion coefficient
- Permeability
- Thermal conductivity
- Viscosity

Electronic, optical, and magnetic properties

- Electron density distribution electrical moments
- Polarizabilities, hyperpolarizabilities
- Optical spectra
- Dielectric properties
- Piezoelectric properties
- Electrostatic potential
- Spin density distribution, magnetic moments
- Energy band structure metal, semiconductor, insulator, superconductor
- Band gaps, band offsets at hetero-junctions
- Ionization energies and electron affinities
- Work function



MD's Technology Platform

MedeA's Three Tier Architecture









www.materialsdesign.com