materials design

Materials Properties and Optimization through Computations

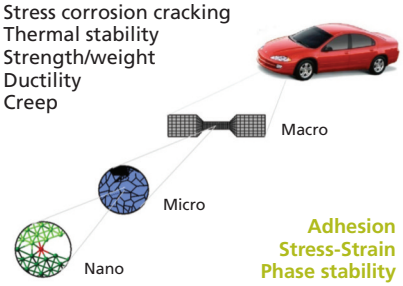
Materials Design is a leading provider of software and consulting services to the materials R&D field. Our capabilities focus on the quantitative prediction of materials properties of direct value in the engineering process.

We enable materials engineers and scientists to improve the performance and reliability of existing materials and to design novel materials by providing:

- *Property prediction where experiments are time consuming, expensive or unfeasible*
- *Interpretation of experiments and the ability to resolve conflicting data*
- *Better fundamental understanding of materials behavior*

Connecting atomic-scale with performance and reliability

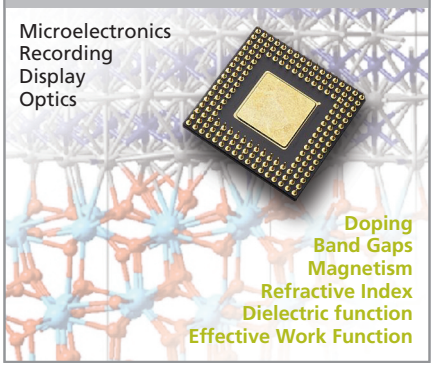
Stress corrosion cracking
Thermal stability
Strength/weight
Ductility
Creep



Adhesion
Stress-Strain
Phase stability
Grain boundaries
Thermal expansion

Controlling functional materials on the atomic scale

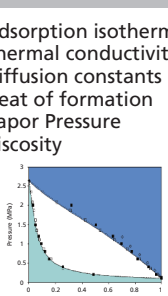
Microelectronics
Recording
Display
Optics



Doping
Band Gaps
Magnetism
Refractive Index
Dielectric function
Effective Work Function

Predicting thermodynamic and transport properties

Adsorption isotherms
Thermal conductivity
Diffusion constants
Heat of formation
Vapor Pressure
Viscosity



Chemical reactivity
Thermodynamic functions
Pathways and activation barriers

Materials Design's technology and expertise fosters materials innovation for application areas including transportation, energy, microelectronics, display, recording technologies and chemical engineering.

Light-weight alloys[1], Ni-based alloys, steels, zirconium[2], glass-ceramics, hard materials

CMOS with high-k dielectrics[3], hydrogen storage materials[4], battery materials, catalysts[5]

Refrigerants, lubricants, specialty chemicals, zeolites for sorption and separation, oil and gas production[6]

*Visit our website **www.materialsdesign.com** or contact your local Materials Design office for further information.*

References:

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2. *Effect of Impurity and Alloying Elements on Zr Grain Boundary Strength from First-Principles Computations, Christensen et al., Paper 2165, Proceedings of Top Fuel 2009 Conference, Paris, France (2009)*
3. *Interfacial oxygen and nitrogen induced dipole formation and vacancy passivation for increased effective work functions in TiN/HfO_2 gate stacks, Hinkle et al., Appl. Phys. Lett. 96, 103502 (2010)*
4. *Crystal structure and thermodynamic stability of the lithium alanates $LiAlH_4$ and Li_3AlH_6, Løvvik et al., Phys. Rev. B 69, 134117 (2004)*
5. *H. Toulhoat, Patent No. US 6,799,089 B2, Sep 28 2004*
6. *Thermodynamic behavior of the CO_2 + SO_2 mixture: experimental and Monte Carlo simulation studies, Lachet et al., Energy Procedia 1, 1641 (2009)*

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