CalSimu Tech

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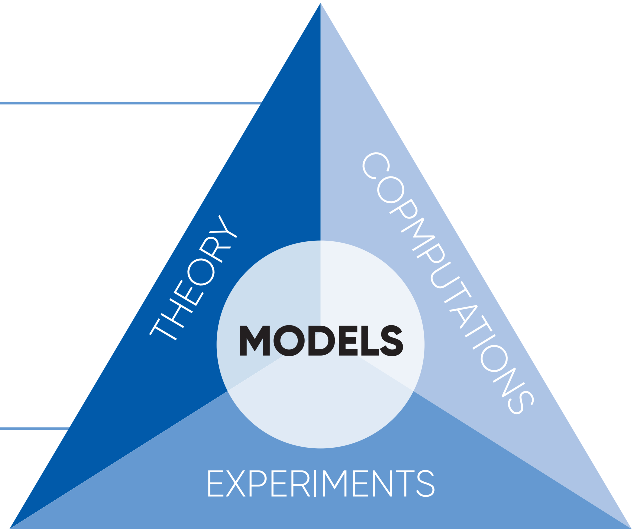
One can probe materials behavior in three ways:

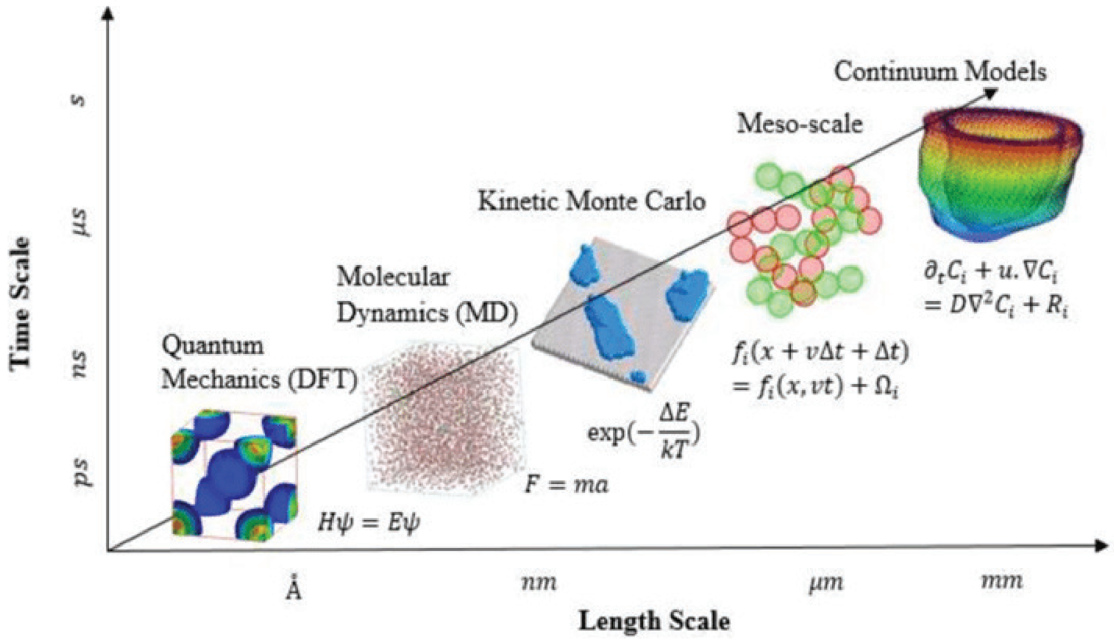
1. Theory
2. Computations » Expertise of this startup.
3. Experiment



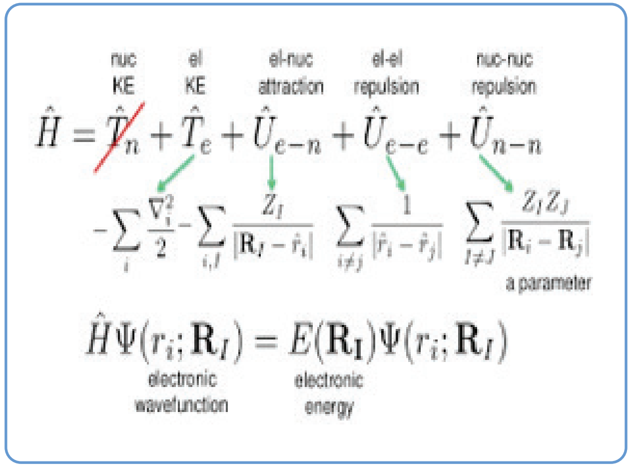
Computational Materials Science

"The application of computational tools to materials discovery, characterization, design and optimization."
(solving quantum mechanical equations for atoms.)

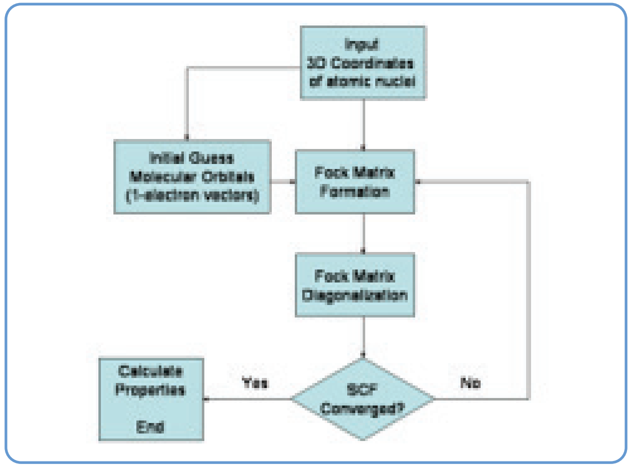
Length & time scales in scientific modeling



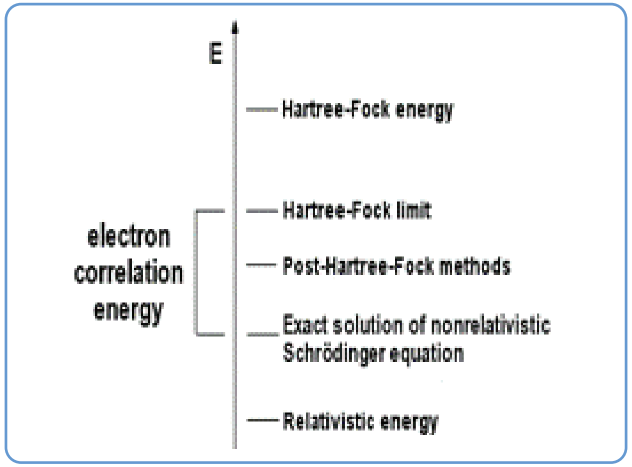
History of quantum mechanical computations



Schroedinger equation to describe electrons-protons



Hartree-Fock flowchart to compute Schroedinger equation



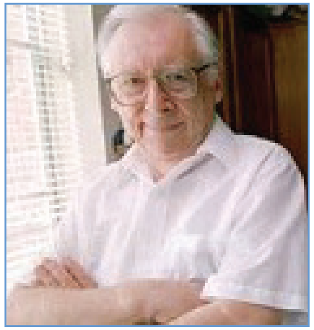
Ab-initio electronic structure methods in terms of energy

Time-lapse

Erwin Schroedinger
(1926)

Hartree
(1935)

Fock
(1935)



John Pople
Gaussian
(1998)

Walter Kohn
DFT Equations
(1998)

Who are using Computational Materials Science?

SAMSUNG

BOSCH Invented for life

LG

Argonne NATIONAL LABORATORY

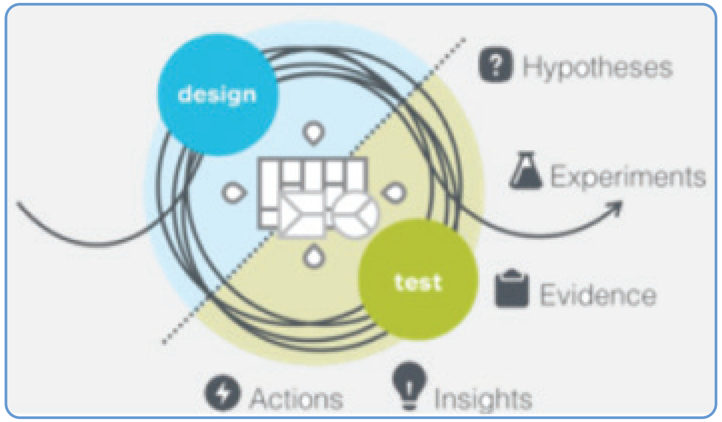
Almost all advanced research centers in the world

Why using Computational Materials Science?

Experimental steps must be designed and executed to save time and money.

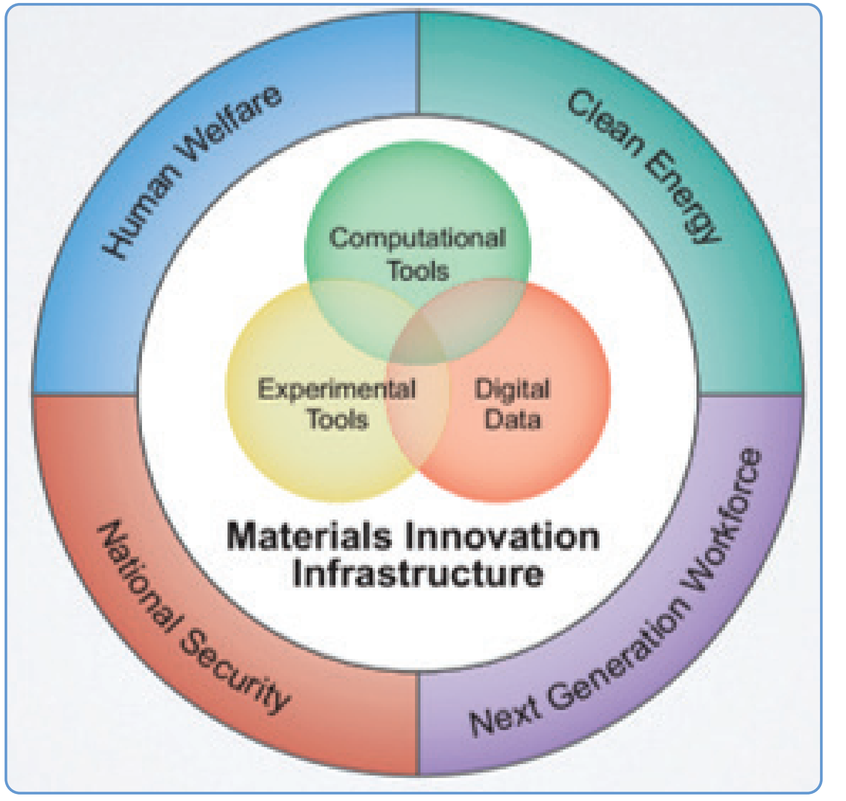
In **CMS**, lengthy experimental steps are replaced by computer modeling to save both **Money** and **Time**.

Modern computations are **cheap** yet **powerful**.



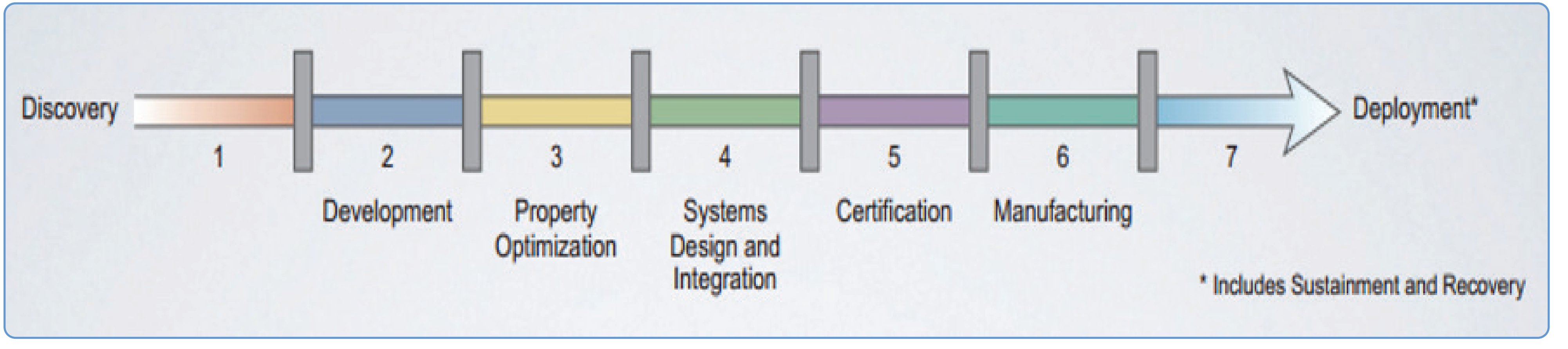
CMS

- » Drives innovation and discovery
- » Addresses international goals
- » Brings new and optimized products to market
- » Trains next-generation workforce



CMS in Industry

Global competitiveness of manufacturing firms requires accelerated materials development and deployment.



CMS can compress development pipeline by eliminating laborious, costly, and lengthy experimental "trial and error".

Validated computational models to perform	
1	Prototyping
2	Screening
3	Materials Selection
4	Materials Design
5	Failure Analysis
6	Virtual Analysis
7	Optimization
8	Reliability Testing

Our main expertise:

Predict materials properties without using experimental results.

Research Methodology Capabilities and Skills:

- Development of screening criteria.
- In-depth analysis of bottlenecks in material performance.
- Molecular dynamics and force field development.
- Ab-initio thermodynamics.
- Ab-initio spectral benchmarking and analysis.
- High-throughput screening of materials.

Research Procedure

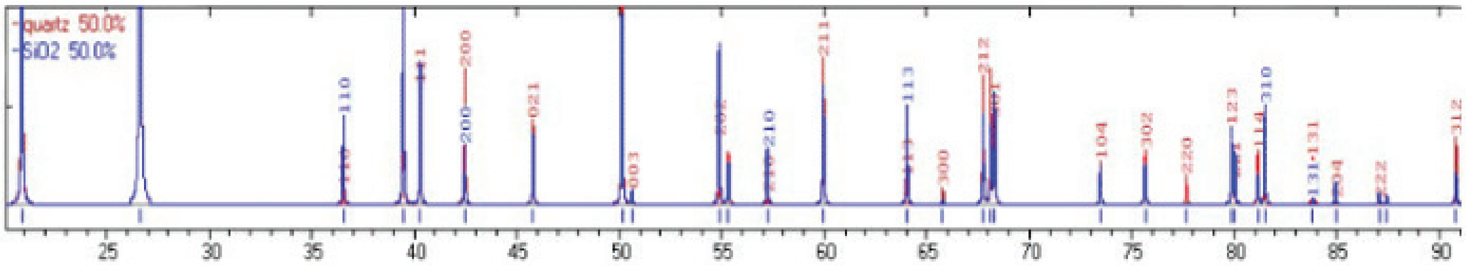
Break device into known materials structures — **Model atomic structure of all materials**

Pre-process to create input files for computations — **Run computations to solve Schrodinger equations**

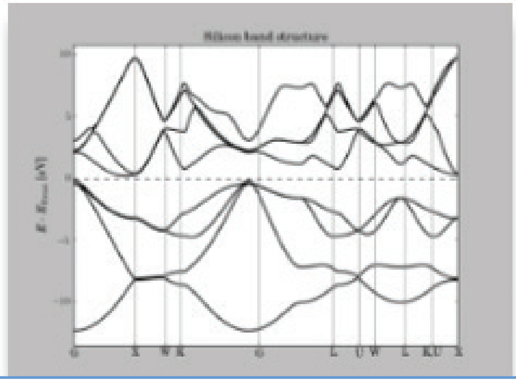
Post-process to extract raw data from output files — **Analyze and Propose materials properties**

Sample of Previous Results

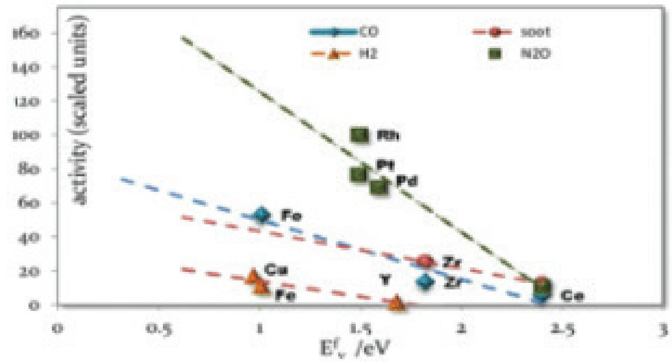
simulation of X-ray diffraction patterns to verify synthesized materials



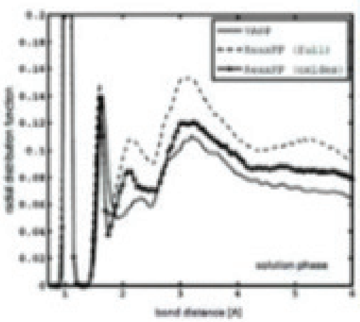
prediction of band structures & band gaps

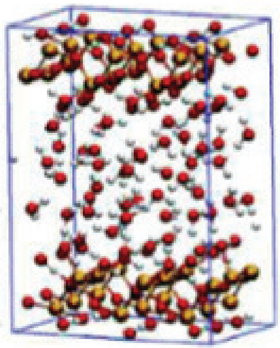


detect chemical & catalytic activities

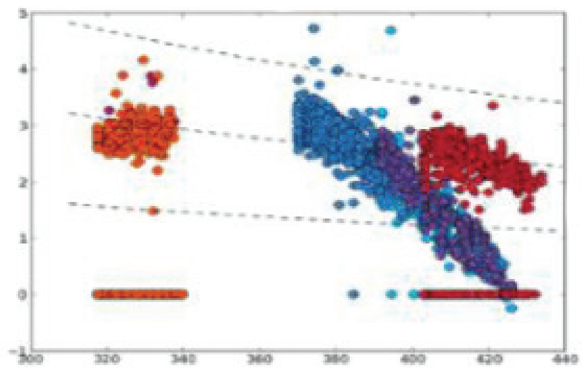


analyze surfaces and adsorbates





screening of battery capacities



Thank You!