Electronic Structure Theory Overview

From Electronic-Structure Theory to Material Science:
Thermodynamics and Statistical Mechanics
from First Principles

Theoretical Concepts and Some Examples (Results)

1. Electronic-Structure Theory
2. *Ab initio* Atomistic Thermodynamics
3. Molecular Dynamics
4. Kinetic Monte Carlo Approach
Dirac: “The underlying physical laws necessary for the mathematical theory of a large part of physics and the whole of chemistry are thus completely known, and the difficulty is only that the exact application of these laws leads to equations much too complicated to be soluble. It therefore becomes desirable that approximate practical methods of applying quantum mechanics should be developed, which can lead to an explanation of the main features of complex atomic systems without too much computation.”

Modeling Materials Properties and Functions: The Many-Body Schrödinger Equation

\[(\hat{T}^e + \hat{T}^{ion} + \hat{V}^{e-e} + \hat{V}^{e-ion} + \hat{V}^{ion-ion})\Psi = E\Psi\]

With:
\[
\Psi(\mathbf{r}_1, \cdots \mathbf{r}_N; \mathbf{R}_1, \cdots \mathbf{R}_M)
\]

\[
\hat{T}^e = \sum_{k=1}^{N} \frac{\mathbf{p}_k^2}{2m}
\]

\[
\hat{T}^{ion} = \sum_{l=1}^{M} \frac{\mathbf{p}_l^2}{2M_l}
\]

\[
\hat{V}^{e-e} = \frac{e^2}{r_{k,k'}}
\]

\[
\hat{V}^{ion-ion}(\mathbf{r}_k, \mathbf{R}_l) = \sum_{k=1}^{N} \sum_{l=1}^{M} \mathbf{v}^{ion}_{\mathbf{R}_l}(||\mathbf{r}_k||)
\]

Where \(\Phi\) are solutions of the “electronic Hamiltonian”:

\[
\Psi(\mathbf{r}_1, \cdots \mathbf{r}_N; \mathbf{R}_1, \cdots \mathbf{R}_M) = \sum_{\nu} \Lambda_{\nu}(\{\mathbf{R}_l\}) \Phi_{\nu,\{\mathbf{R}_l\}}(\{\mathbf{r}_k\})
\]

frequently (commonly) applied approximations:
- neglect non-adiabatic coupling (terms of order \(m/M_l\))
- keep only \(\Lambda_0\)

\(\longrightarrow\) the dynamics of electrons and nuclei decouple

Born-Oppenheimer Approximation

\[
\Psi(\mathbf{r}_1, \cdots \mathbf{r}_N; \mathbf{R}_1, \cdots \mathbf{R}_M) = \sum_{\nu} \Lambda_{\nu}(\{\mathbf{R}_l\}) \Phi_{\nu,\{\mathbf{R}_l\}}(\{\mathbf{r}_k\})
\]

Where \(\Phi\) are solutions of the “electronic Hamiltonian”:

\[
H^{e}_\{\mathbf{R}_l\} \Phi_{\nu,\{\mathbf{R}_l\}}(\{\mathbf{r}_k\}) = E^{e}_\nu,\{\mathbf{R}_l\} \Phi_{\nu,\{\mathbf{R}_l\}}(\{\mathbf{r}_k\})
\]

\[
H^e = T^e + V^{e-e} + V^{e-ion}
\]

\(\hat{\Phi}\) are solutions of the “nuclear Hamiltonian”:

\[
\hat{\Phi}(\mathbf{r}_1, \cdots \mathbf{r}_N; \mathbf{R}_1, \cdots \mathbf{R}_M) = \sum_{\nu} \Lambda_{\nu}(\{\mathbf{R}_l\}) \Phi_{\nu,\{\mathbf{R}_l\}}(\{\mathbf{r}_k\})
\]

\[
H^{ion} = \sum_{l=1}^{M} \frac{\mathbf{p}_l^2}{2M_l}
\]

\[
\hat{V}^{ion-ion}(\mathbf{r}_k, \mathbf{R}_l) = \sum_{k=1}^{N} \sum_{l=1}^{M} \mathbf{v}^{ion}_{\mathbf{R}_l}(||\mathbf{r}_k||)
\]
Some Limits of the Born-Oppenheimer Approximation

It does not account for correlated dynamics of ions and electrons. For example:

- polaron-induced superconductivity
- dynamical Jahn-Teller effect at defects in crystals
- some phenomena of diffusion in solids
- non-adiabaticity in molecule-surface scattering and chemical reactions
- relaxation and transport of charge carriers ($e^-$ or $h$)
- etc.

These limits can be severe. Nevertheless, we will use the BO approximation in the following.

How can we solve:

\[
H_e^{(R_1)} \Phi_{\nu,\{R_1\}}(r_k) = E_e^{(R_1)} \Phi_{\nu,\{R_1\}}(r_k)
\]

\[
H^e = T^e + V^{e-e} + V^{e-\text{ion}}
\]
The Hohenberg-Kohn Theorem (1964)

Set of non-degenerate ground-state wave functions $\Phi$ of arbitrary $N$-electron Hamiltonians. Set of particle densities $n(r)$ belonging to non-degenerate $N$-electron ground states.

The dashed arrow is not possible. Thus, here is a one-to-one correspondence between $\Phi$ and $n(r)$.

Comparison of Wave-Function and Density-Functional Theory

$\langle \Phi | H^e | \Phi \rangle$  $\rightarrow$  $\Phi_0$  \hspace{1cm}  $E_v[n]$  $\rightarrow$  $E_0$

Schrödinger

$\Phi(\{r_i\})$  $\sim 10^{23}$ Variables
Comparison of Wave-Function and Density-Functional Theory

The energy of the ground state of a many-electron system:

$$E_0 \{\{R_i\}\} = \text{Min}_{\Phi} <\Phi|H^e|\Phi>$$

Hohenberg and Kohn (1964): The functional

$$n(r) = n[\Phi] = <\Phi|\sum_i \delta(r-r_i)|\Phi>$$

can be inverted, i.e.,

$$\Phi(r_1, r_2, \ldots, r_N) = \Phi[n(r)]$$.

This implies:

$$E_0 \{\{R_i\}\} = \text{Min}_{n(r)} E_{\{R\}} [n]$$

Density Functional Theory
The Kohn-Sham Ansatz of Density-Functional Theory

- **Kohn-Sham (1965):** Replace the original many-body problem by an independent electron problem that can be solved!

\[ E_v[n] = T_s[n] + \int v(\mathbf{r}) n(\mathbf{r}) \, d^3\mathbf{r} + E^{\text{Hartree}}[n] + E^{\text{xc}}[n] \]

- With \( T_s[n] \) the kinetic energy functional of independent electrons, and \( E^{\text{xc}}[n] \) the unknown functional.
- The challenge is to find useful, approximate xc functionals.

Kohn and Sham (1965):

\[ E_v[n] = T_s[n] + \int v(\mathbf{r}) n(\mathbf{r}) d^3\mathbf{r} + E^{\text{Hartree}}[n] + E^{\text{xc}}[n] \]

with \[ E^{\text{Hartree}}[n] = \frac{1}{2} \frac{e^2}{4\pi\varepsilon_0} \iint \frac{n(\mathbf{r}) n(\mathbf{r}')}{|\mathbf{r} - \mathbf{r}'|} \, d^3\mathbf{r} d^3\mathbf{r}' \]

And \( T_s[n] \) the functional of the kinetic energy of non-interacting electrons. \( E^{\text{xc}}[n] \) contains all the unknowns.

At fixed electron number \( N \) the variational principle gives

\[ \delta \left\{ E_v[n] - \mu \left( \int n(\mathbf{r}) d^3\mathbf{r} - N \right) \right\} = 0 \]

or \[ \frac{\delta E_v[n]}{\delta n} = \mu = \frac{\delta T_s[n]}{\delta n(\mathbf{r})} + v^{\text{eff}}(\mathbf{r}) \]

Kohn-Sham equation
Kohn and Sham (1965):

\[ v_{\text{eff}}(r) = v(r) + \frac{e^2}{4\pi \varepsilon_0} \int \frac{n(r')}{|r - r'|} \, d^3r' + \frac{\delta E_{\text{xc}}[n]}{\delta n(r)} \]

Because \( T_s[n] \) is the functional of non-interacting particles, we effectively restrict the allowed densities to those that can be written as

\[ n(r) = \sum_{i=1}^{N} |\varphi_i(r)|^2 \]

This implies:

\[ \left\{ -\frac{\hbar^2}{2m} \nabla^2 + v_{\text{eff}}(r) \right\} \varphi_i(r) = \varepsilon_i \varphi_i(r) \]

\( v_{\text{eff}}(r) \) depends on the density that we are seeking.

\[ T_s[n] = \sum_{k=1}^{N} \langle \varphi_k \left| -\frac{\hbar^2}{2m} \nabla^2 \right| \varphi_k \rangle, \]

\[ = \sum_{k=1}^{N} \varepsilon_k - \int v_{\text{eff}}[n_{\text{in}}](r)n(r) \, d^3r. \]

---

**Solving the Kohn-Sham Equations**

- Structure, types of atoms
- Guess input electron density
- Solve KS eqs. (e.g. FHI-aims, FLAPW, or ...)
- Build the new density
- Self-consistent?
- Output:
  - Total energy, forces, ...
  - Kohn-Sham eigenvalues

---

**The self-consistent field method**

**Initial Guess**

\( n^0(r), \varepsilon^0(r) \)

**Calculate Effective Potential**

\[ V_{\text{eff}}(r) = V_{\text{ext}}(r) + V_{\text{core}}(r) + V_{\text{xc}}[n^0, n^0] \]

**Solve KS Equations**

\[ \left( -\frac{\hbar^2}{2m} + V_{\text{eff}}(r) \right) \psi_i(r) = \varepsilon_i \psi_i(r) \]

**Calculate Electron Density**

\[ n^0(r) = \sum_i |\psi_i(r)|^2 \]  

**k-point summation**

**update the geometry**

**mixing**

**Self-consistent?**

Yes

No

**Output Quantities**

Total energy, forces, etc.
**The xc Functional**

$T_s$, $E_{\text{Hartree}}$, and $E_{\text{xc}}$ are all *universal* functionals in $n(r)$, i.e., they are independent of the special system studied. (general theory: see the work by Levy and Lieb)

$$E_{\text{xc}}[n] = \int \epsilon_{\text{xc}}[n] n(r) d^3r = E_{\text{xc-LDA}}[n] + O(\nabla n)$$

$E_{\text{xc-LDA}} = \int \epsilon_{\text{xc-jellium}}(n) n(r) d^3r$

The $\epsilon_{\text{xc-jellium}}(n)$ function is the local-density approximation

DFT Summary -- in Practice

**Hohenberg-Kohn theorem**: It is exact.

**Kohn-Sham theory**: Introducing $E_{\text{xc}}[n]$ and its functional derivative. … My conclusion: It is probably not possible to write down $E_{\text{xc}}[n]$ as a closed mathematical expression.

Here is how the *exact functional* looks:

(*) In general, a “functional” is defined in terms of an “algorithm”, i.e. a self-contained step-by-step set of operations.
The success of DFT proves that “simple” approximations to the exchange-correlation functional can provide good results – if one knows what one is doing.

Hohenberg-Kohn theorem: It is exact.

Kohn-Sham theory: Introducing $E_{xc}[n]$ and its functional derivative. … My conclusion: It is probably not possible to write down $E_{xc}[n]$ as a closed mathematical expression.

Here is how the exact functional(*) looks:
ground-state density $\leftrightarrow$ ground-state many-electron wave function $\leftrightarrow$ many-electron hamiltonian $\rightarrow$ total energy and all other observables.

The success of DFT proves that “simple” approximations to the exchange-correlation functional can provide good results – if one knows what one is doing.

(*) In general, a “functional” is defined in terms of an “algorithm”, i.e. a self-contained step-by-step set of operations.
Perdew’s Dream: Jacob’s Ladder in Density-Functional Theory

The exchange-correlation functional

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<tr>
<th>Accuracy</th>
<th>Favorite</th>
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<td>5</td>
<td>unoccupied $\psi_i(r)$, EX + cRPA, as given by ACFD</td>
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<td>$n(r)$, Local-Density Approximation</td>
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$\tau(r)$: Kohn-Sham kinetic-energy density
EX: exact exchange: $E_x = -\frac{1}{2} \sum_{\text{occ}} \int dr dr' \psi_i^*(r) \psi_m(r) \psi_i^*(r') \psi_m(r') / |r - r'|$

$cRPA$: random-phase approximation for correlation
ACFD: adiabatic connection fluctuation dissipation theorem

Bohm, Pines (1953); Gell-Mann, Brueckner (1957); Gunnarsson, Lundqvist (1975, 1976); Langreth, Perdew (1977); X. Ren, P. Rinke, C. Joas, and M. S., Invited Review, Mater. Sci. 47, 21 (2012)

Perdew's Dream: Jacob’s Ladder in Density-Functional Theory

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Ab initio Atomistic Thermodynamics

Assumption of thermodynamic equilibrium
This means that any information about time-scales is lost. We look at the system after infinite time.

Note that in reality the kinetics *can* be very slow; an extreme example is C-diamond $\leftrightarrow$ graphite.

Sometimes it is important (and possible) to define a constrained equilibrium.
### Thermodynamics (A Brief Reminder)

#### Thermodynamic potentials:

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<th>Expression</th>
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<td>Internal energy</td>
<td>$U(S, V) = E^{\text{tot}} + U^{\text{vib}}$</td>
</tr>
<tr>
<td>Enthalpy</td>
<td>$H(S, p) = U + pV$</td>
</tr>
<tr>
<td>(Helmholtz) free energy</td>
<td>$F(T, V) = U - TS$</td>
</tr>
<tr>
<td>Gibbs free energy</td>
<td>$G(T, p) = U - TS + pV$</td>
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$E^{\text{tot}}$ contains energy contributions from chemical binding (structure) as well as electronic excitations, if present. $U^{\text{vib}}$ is the energy of vibrations. For polyatomic systems $E^{\text{tot}}$ and $U^{\text{vib}}$ are best calculated by DFT.

At thermodynamic equilibrium the corresponding thermodynamic potential assumes its minimum.

Chemical potential $\mu = (\partial G / \partial N)_{T, p} = \mu = \text{the cost to remove a particle from the system.}$
The first (convincing) DFT calculations: Stability of crystals and crystal phase transitions

\[ \begin{array}{c|c|c|c|c|c} \text{Volume} & 0.6 & 0.7 & 0.8 & 0.9 & 1.0 & 1.1 \\ \hline \text{Total energy (Ryd./atom)} & -7.84 & -7.86 & -7.88 & -7.90 & -7.92 \\ \end{array} \]

- Silicon
- Diamond
- B-tin

see also:
V. L. Moruzzi, J. F. Janak, and A. R. Williams
Calculated Electronic Properties of Metals
Pergamon Press (1978)

Ab Initio Atomistic Thermodynamics
Effect of a Surrounding Gas Phase on Surface Structure and Composition

Surface in Contact with a One-Component Gas Phase – Example: O₂ @ Pd

\[ \gamma_{\text{surf.}} = \frac{1}{A} \left[ G(N_O, N_{\text{Pd}}) - N_O \mu_O - N_{\text{Pd}} \mu_{\text{Pd}} \right] \]

\[ N_O = \text{# of O atoms in the system} \]
\[ N_{\text{Pd}} = \text{# of Pd atoms (substrate) in the system} \]

Concept of thermodynamic reservoirs:
1) The environment can give and take O atoms at an energy \( \mu_O = \frac{1}{2} \mu_{O_2} \)

\[ \mu_O(T, p) = \frac{1}{2} \mu_{O_2}(T, p^0) + \frac{1}{2} k_B T \ln\left(\frac{p}{p^0}\right) \]

2) Also the bulk of the substrate is practically of infinite size and acts as a reservoir for the Pd atoms: \( \mu_{\text{Pd}} = g_{\text{Pd bulk}} \)

Oxide Formation on Pd(100)

M. Todorova et al.,
Surf. Sci. 541, 101 (2003);
K. Reuter and M. Scheffler,
Oxide Formation on Pd(100)

![Graph showing the phase diagram for oxide formation on Pd(100)]

InAs/GaAs(001) quantum dots close to thermodynamic equilibrium

*G. Costantini et al. APL 82 (2003)*

![ STM images of InAs/GaAs(001) quantum dots ]

(a) STM topography of a large island.


c), d) High-resolution views of the (110) and (111) side facets.

Also:

J. Marquez et al., APL 78 (2001);
Y. Temko et al., APL 83 (2003).
Summary *Ab Initio* Atomistic Thermodynamics

- Calculate *free energies* by DFT.
- Exploit thermodynamic equilibria and the concept of thermal reservoirs (atomic chem. potentials).

- Concentration of point defects at finite $T$
- Surface structure and composition in realistic environments
- Order-order and order-disorder phase transitions
- Equilibrium shape of (nano) crystals

Limitations:

-- The accuracy of the xc functional (with respect to $k_B T$)
-- “only” thermodynamic equilibrium

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Theoretical Concepts and Some Examples (Results)

✓ 1. Electronic-Structure Theory (Part I)
✓ 2. *Ab initio* Atomistic Thermodynamics
  3. Molecular Dynamics
  4. Kinetic Monte Carlo Approach
Brief History of MD

First MD simulation: B.J. Alder and T.E. Wainwright, 1956 - hard sphere liquid, phase transition

First MD simulations with a continuous potential: G.H. Vineyard et al, 1959 -- radiation damage simulation with a pair potential
A. Rahman, 1964 - Lennard-Jones liquid

First MD with DFT energetics: R. Car and M. Parrinello, 1985 – Si crystal

Computational cost is almost always dominated by the cost of the force call (evaluating $E_{\text{tot}}$ and $dE_{\text{tot}}/dR$), not by the integrator itself.

Stability of Secondary Structures

structure of proteins (peptide chains):

amino group

peptide bond

carboxyl group

Secondary structure

sheets

turns

helices

Tertiary structure

$R = \text{CH}_3$

= alanine
Role of vdW Interaction on (Un)folding; Ac-Ala_{15}LysH^+

http://www.youtube.com/watch?v=Y_7G8s26zzw  
PRL 106, 118102 (2011)

What Did We Learn from Studying Polypeptides?

Density-functional theory (PBE+vdW) is able to:

- Predict geometry and properties, analyze stability and unfolding:
  - hydrogen bonding,
  - vdW interaction, and
  - vibrational entropy.

- Verification of structure predictions against experiment (vibrational spectroscopy).

M. Rossi, V. Blum, et al., JPCL 1 (2010).
A Tkatchenko, M Rossi, V Blum, J Ireta, M.S., PRL 106, 118102 (2011)
http://www.youtube.com/watch?v=Y_7G8s26zzw
Au_{13} at Room Temperature visiting many metastable structures

Ab Initio Melting Curve of Fe as Function of Pressure

D. Alfe, M. J. Gillan, and G. D. Price
NATURE 401 (1999)
Possibilities and Limitations of MD

With force fields (no explicit quantum mechanics): $10^3 - 10^4$ atoms are possible on a single processor.

Much larger systems are possible via parallelization: several million atoms are now routine; billions of atoms are possible.

With DFT energies: just ~100 atoms (soon 1000)

Problems:
- Accuracy of the interatomic interaction
- Length scale – (still) not macroscopic
- Time scale - limited to ~ 1 ms (with simple potentials) and with DFT energies up to 1 ns
- Quantum dynamical effects of the nuclei are typically ignored.
- Non adiabatic dynamics not treated properly

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**Kinetic Monte Carlo:**
Coarse-Graining Molecular Dynamics

\[ \langle \Delta t \rangle = \frac{1}{k_{TST}} \]

Molecular Dynamics of Co on Cu(001): The whole trajectory.

- *ab initio MD*: up to 100 ps

Kinetic Monte Carlo simulation: Coarse-grained hops.

- *ab initio kMC*: up to minutes
The system vibrates in a multi-dimensional basin. Occasionally it escapes, crossing through a dividing surface to a new basin. This behavior characterizes solid-state diffusion, chemical reactions at surfaces, as well as many other systems and properties.

**Molecular Dynamics of Co on Cu(001):** The whole trajectory.
- **ab initio MD:** up to 50 ps

**Kinetic Monte Carlo simulation:** Coarse-grained hops.
- **ab initio kMC:** up to minutes

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**Master-Equation**

for Molecular Simulations over Long Time Periods

\[ p_n(t) = \sum_m \left[ w_{nm}(t)p_m(t) - w_{mn}(t)p_n(t) \right]. \]

The probability to find at time \( t \) the metastable atomic configuration (conformation) \( n \), follows from a gain term (transitions \( m \to n \)) and a loss term (transitions \( n \to m \)).

When the number of conformations is large, the direct solution of the master equation becomes impractical.

Kinetic Monte Carlo. This is a very efficient, numerical solution of the master equation.
Flowchart of A Kinetic Monte-Carlo Simulation

START

Get two random numbers \( r_1, r_2 \in [0,1] \)

determine all possible processes \( \{ i \} \) for the present configuration and build a list of the rates: \( \{ \Gamma^{(i)} \} \)

Calculate \( R = \sum_i \Gamma^{(i)} \) and select process “\( k \)”: 

\[
\frac{\sum_{i=1}^{k-1} \Gamma^{(i)}}{\sum_{i=k+1}^{N} \Gamma^{(i)}} \leq r_1 R \leq \frac{\sum_{i=1}^{N} \Gamma^{(i)}}{\sum_{i=k+1}^{N} \Gamma^{(i)}}
\]

update the clock 

\( t \rightarrow t - \ln(r_2)/R \)

Execute process number “\( k \)”, i.e. update the configuration

END

A. Bortz, M. Kalos, and J. Lebowitz, *J. Comp. Phys.* 17, 10 (1975)

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kMC Summary

- kMC is a numerical solution of the master equation.
- It gives essentially the same information as MD, but can simulate time spans \( >10^{12} \) times longer.
- It can be linked to *ab initio* rate processes: free energy barriers, and their \( T \) dependence. Often transition state theory can be applied. Configurational entropy and resulting (kinetic) barriers are obtained by the kMC simulation. .. and more.
- The main challenge for building a reliable kMC simulation is to find all the important processes.

---
Microscopic Processes Controlling The Growth -- Example: III-V Semiconductors

1) deposition of Ga and As  
2) adsorption of Ga  
3) diffusion of Ga  
4) desorption of Ga  
5) adsorption of As$_2$  
6) dissociation of As$_2$  
7) diffusion of As  
8) desorption of As  
9) island nucleation  
10) growth

Theory of The Kinetics of Growth

1) Analysis of all possibly relevant processes using density-functional theory
2) Calculate the rates of all important processes
   \[ \Gamma^{(i)} = \Gamma_0^{(i)} \exp \left( -\Delta E^{(i)} / k_B T \right) \]
3) Statistical approach to describe
   - deposition
   - diffusion
   - nucleation
   - growth
   extended kinetic Monte Carlo
Adsorption, diffusion, island nucleation, and growth of GaAs, studied by *ab initio* kinetic Monte Carlo

1/60 of the full simulation cell
As$_2$ pressure 1.33 x $10^{-8}$ bar
Ga deposition rate = 0.1 ML/s
$T = 700$ K

*P. Kratzer & M. S., PRL 88, 036102 (2002)*

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**Island Density**  
*P. Kratzer & M. S., PRL 88, 036102 (2002)*

As$_2$ pressure  
= 1.33 x $10^{-8}$ bar
Ga deposition rate  
= 0.1 ML/s

Log$_{10}$ of saturation island density does not increase linearly with $1/T$: Unusual dependence for $T > 600$ K.
Summary: Interacting electrons determine the properties and function of real materials

Important arenas for future theoretical work:

• Non-adiabatic effects, dissipation
• Transport (electrons, ions, heat)
• Thermodynamic phase transitions, e.g. melting
• Modeling the kinetics, e.g. of catalysts or crystal growth (self-assembly and self-organization) – in realistic environments
• Molecules and clusters (incl. bio molecules) in solvents, electrochemistry, fuel cells, external fields
• Correlated systems, e.g. f-electron chemistry
• Big-data analytics (statistical learning, compressed sensing, etc.)

The challenges:

➢ Find ways to control the xc approximation
➢ Develop methods for bridging length and time scales.

The Novel Materials Discovery (NOMAD) Laboratory develops a Materials Encyclopedia and Big-Data Analytics tools for materials science and engineering.

Eight complementary computational materials science groups and four high-performance computer centers form the synergetic core of this Centre of Excellence.
The NoMaD Repository accepts (and requests) in- and output files of all important codes. Currently, the NoMaD Repository contains 3,026,745 entries.

The NoMaD Laboratory
A European Centre of Excellence

http://nomad-repository.eu
also described at youtube.com
Welcome to the NoMaD Repository

The NoMaD (Novel Materials Discovery) Repository was established to host, organize, and share materials data.

NoMaD offers this for free. NoMaD also facilitates research groups to share and exchange their results, inside a single group or between two or more, and to recall what was actually done some years ago.

The NoMaD Repository enables the confirmatory analysis of materials data, their reuse, and repurposing.

Upload of data is possible without any barrier. Results are accepted in their raw format as produced by the underlying code. The only condition is that the list of authors is provided, and code and code version can

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Read more details concerning the upload. Please, register or login to participate.

At present, the repository contains ab initio electronic-structure data from density-functional theory and methods beyond. At a later stage, it will be extended by force-field studies and by experimental data. We also give an outlook on the NoMaD Laboratory that will be dedicated to a Materials Encyclopaedia, as the basis for complex queries and the development of various data-analytics tools.
The NoMaD Repository accepts (and requests) in- and output files of all important codes. Currently, the NoMaD Repository contains 3,026,745 entries.