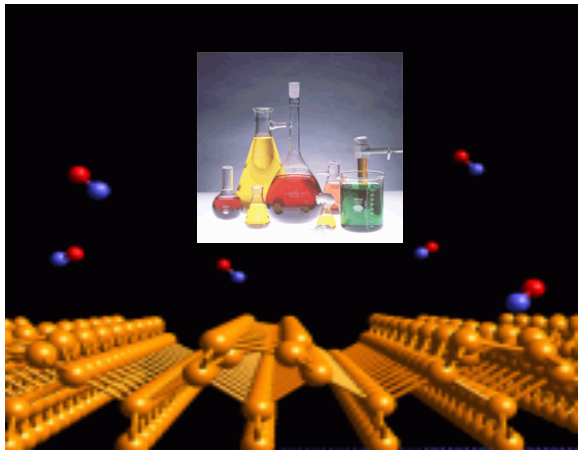
Computational Materials Design: From Molecular Mechanics to Artificial Intelligence

Anatoli Korkin

Nano & Giga Solutions, President
Arizona State University, Adjunct Faculty



Brief professional history

- MS from Mendeleev University of Chemical Technology of Russia
- PhD from Lomonosov Moscow State University
- 10 years researcher in Soviet Union Academy of Science
- 4 years research in Germany: University of Erlangen-Nurnberg and Max-Planck Institute in Muelheim-an-der-Ruhr
- 2 years research at the University of Florida
- 6 years R & D at Motorola, Phoenix, Arizona
- 9 years at Arizona State University
- Short research visits at Dalhousie University, Canada, Tyndall Institute, Ireland, and University of Tokyo, Japan
- 15 years of consulting experience

Research areas

Modeling reaction centers of photosynthetic bacteria
PhD work at Moscow State University

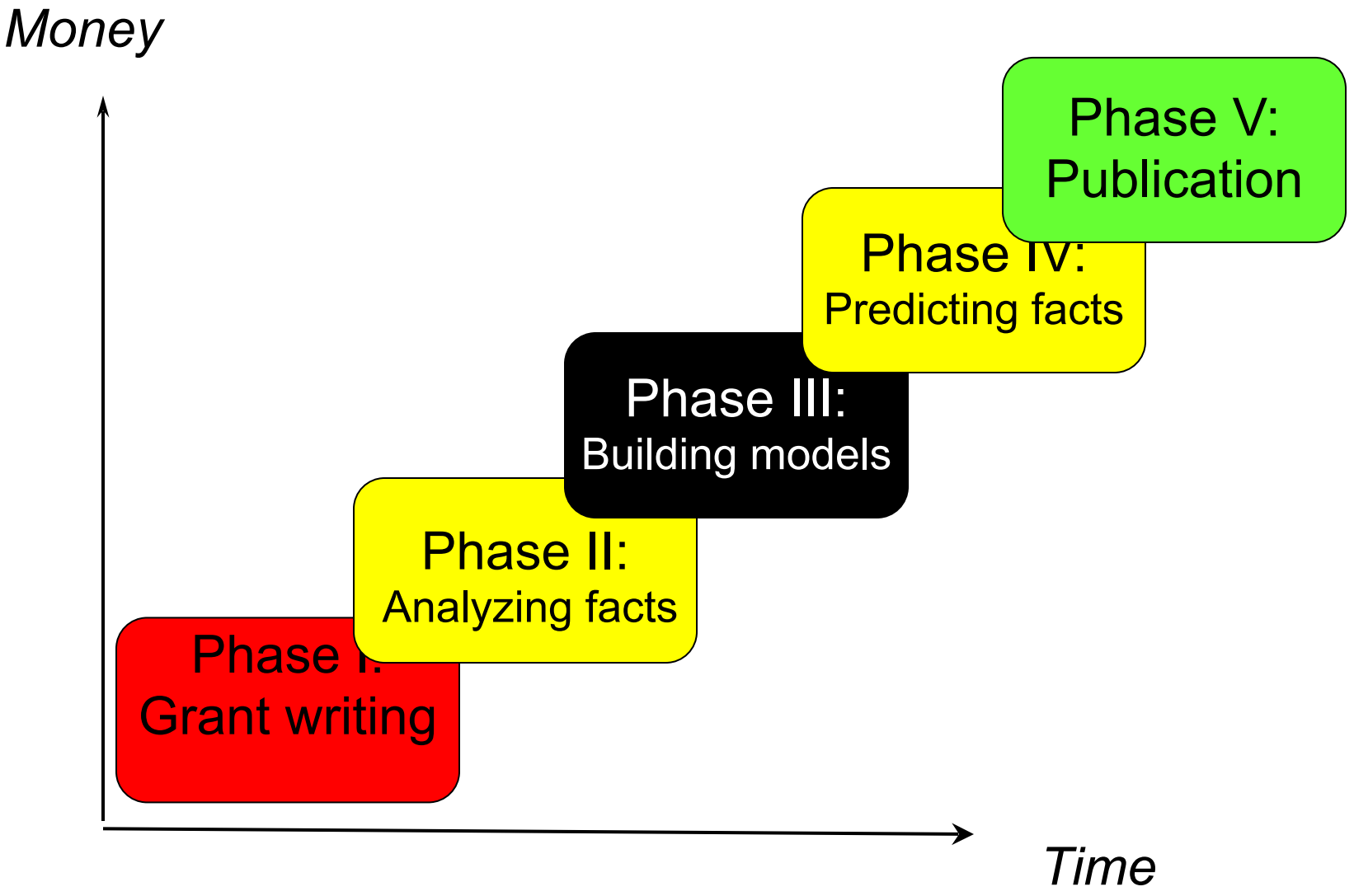
Computational studies of structures and properties of the compounds 1st and 2nd rows
Russian Academy of sciences and Nurnberg University, Germany

Computational studies of biologically active oligopyrroles – models of phytochrome
Max-Planck Institute, Germany

Computational design of advanced propellants and explosives
University of Florida, USA, Dalhousie University, Canada

Computational design of electronic materials and devices
Motorola, USA, University of Tokyo, Japan,Tyndall Institute, Ireland

How we do research



University of the 21st Century – Knowledge Factory

Ancient

Medieval

Modern

Education => Research => Innovations

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Computational Materials Science: General

What computational materials scientists do?
Theory development => Software design => Applications

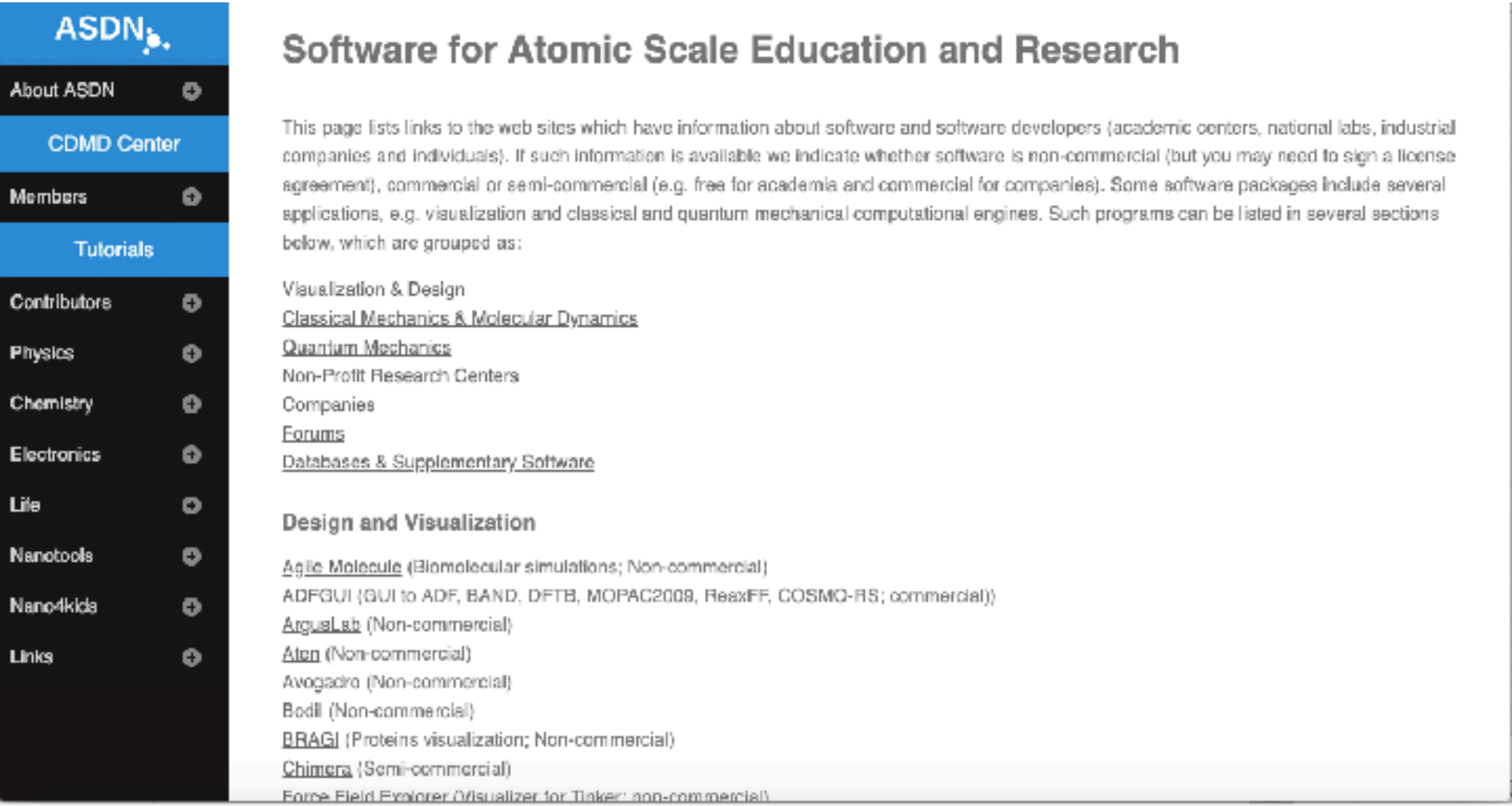
How materials scientists work?
Top down approach: Start from macro scale properties
Bottom up approach: Start from atomic scale structures

Interaction between theory and experiment:
Design of novel materials with desired properties, guidance for reaction paths and technology, atomic scale knowledge of materials and properties as a guidance for experiments.

Knowledge base for computational materials sciences
General: Quantum mechanics, molecular mechanics and dynamics, applied mathematics, statistical methods, computer science

Where computational materials scientists work?
Academia: chemistry, physics, biology, engineering
Industry: pharma, chemicals, construction, electronics

Computational Materials Science: Software



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Computational Materials Science: Lectures

The unexpected behavior of nanoworld

https://asu-teacherscollege.wistia.com/medias/s91tu3bqxu

Feeding biology with electrons

https://www.youtube.com/watch?v=qEvmKGBFpRs

Nanotechnology pathways to next generation photovoltaics

https://www.youtube.com/watch?v=g9q2WBRe4jQ

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Computational Materials Science: Online

Computational materials science, M.Sc. (Sweden, Malmo University)

https://www.mastersportal.com/studies/39616/computational-materials-science.html

Quantum world, course offered by Harvard

https://opencourser.com/course/ia8xfq/edx-the-quantum-world

Quantum mechanics of molecular structures offered by University of Tokyo

https://opencourser.com/course/xdbaim/edx-quantum-mechanics-of-molecular-structures

Atomistic computer modeling of materials offered by MIT

https://ocw.mit.edu/courses/materials-science-and-engineering/3-320-atomistic-computer-modeling-of-materials-sma-5107-spring-2005/

Computational materials science and engineering by Nanohub.org

https://nanohub.org/resources/22124#series

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Molecular mechanics and dynamics

$$E_{total} = E_{bond} + E_{angle} + E_{torsion} + E_{electro} + E_{vdw}$$

Advantage: simplicity, computational efficiency, possibility to compute larges systems

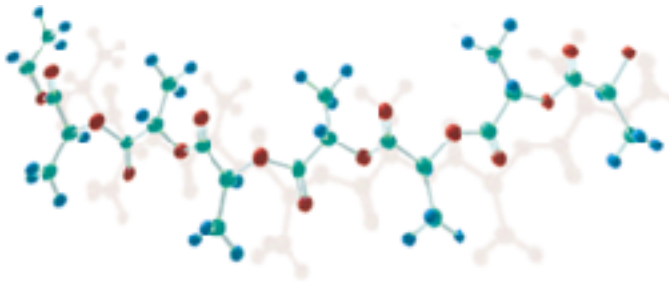
Deficiency: description of phenomena where quantum mechanical effects are essential and can not be emulated by classical force-field potentials

Applications: large systems such as polymers, proteins, DNA, amorphous materials, education, initial structures for subsequent quantum mechanical calculations

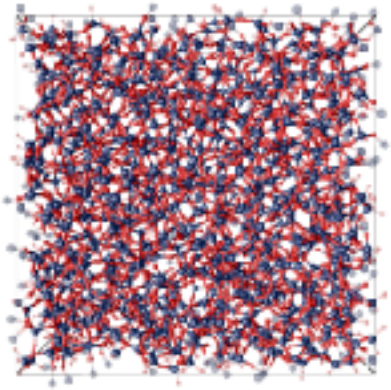
Structure optimization: Simulated annealing, Monte-Carlo, evolutionary algorithms

Peptides

Polymers



Glasses



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Computational design of biomolecules: Samples

Progress in computational protein design
Shaun M.Lippow , Bruce Tidor
Current Opinion in Biotechnology, V 18 (2007) 305-311

Computational Design of Ligand Binding Proteins with High Affinity and Selectivity
Christine E. Tinberg, et al. Nature 501 (2013) 212–216.

Design of a Novel Globular Protein Fold with Atomic-Level Accuracy
Brian Kuhlman, et al Science, B 302 (2003) 1364-1368

Paradigms for computational nucleic acid design
Robert M. Dirks Milo Lin Erik Winfree Niles A. Pierce
Nucleic Acids Research, Volume 32, 2004 1392–1403

Hartree-Fock and DFT methods

Hartree-Fock method: $\hat{F}(1)\phi_i(1) = \epsilon_i \phi_i(1)$ $\phi_i = \sum_r c_{ri}\chi_r$

$$\hat{F}[\{\phi_j\}](1) = \hat{H}^{\text{core}}(1) + \sum_{j=1}^{N/2}[2\hat{J}_j(1) - \hat{K}_j(1)] \qquad \hat{H}^{\text{core}}(1) = -\frac{1}{2}\nabla_1^2 - \sum_\alpha \frac{Z_\alpha}{r_{1\alpha}}$$

Approximations: 1. Born-Oppenheimer; 2. Non-relativistic. 3. Finite basis set; 4. Wave function – single Slater determinant; 5. Mean-field approximation

DFT: $\left[-\frac{\hbar^2}{2m}\nabla^2 + V_s(\vec{r})\right]\varphi_i(\vec{r}) = \varepsilon_i\varphi_i(\vec{r})$ $n(\vec{r}) \overset{\text{def}}{=} n_s(\vec{r}) = \sum_i^N |\varphi_i(\vec{r})|^2.$

$$V_s(\vec{r}) = V(\vec{r}) + \int \frac{e^2 n_s(\vec{r}')}{|\vec{r} - \vec{r}'|}\,\mathrm{d}^3r' + V_{XC}[n_s(\vec{r})]$$

Advantage: Quantum mechanical nature of molecules considered explicitly

Disadvantage: Accuracy comes with a higher computational costs and complexity

Quantum chemistry tools set

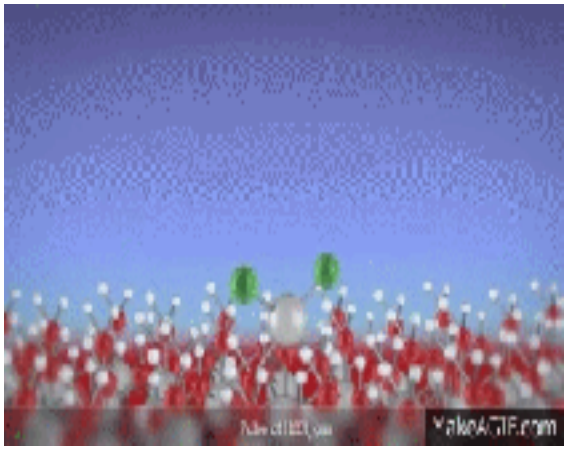
NDDO <= HF => Mueller-Plesset => Coupled-Cluster => CAS SCF

Pseudo-potentials <= LDA <= DFT => GGA => B3LYP => TD-DFT; FT-DFT

Quantum mechanics => QM + Molecular Mechanics + Continuum

Reactions in liquids

Chemical deposition



Catalysis

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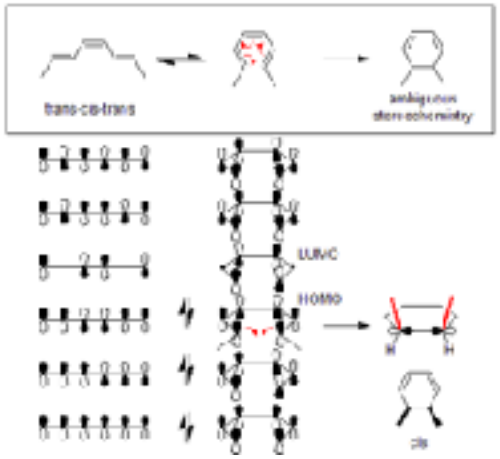
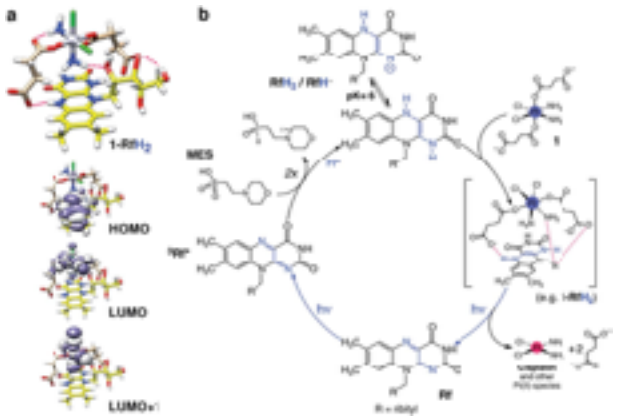
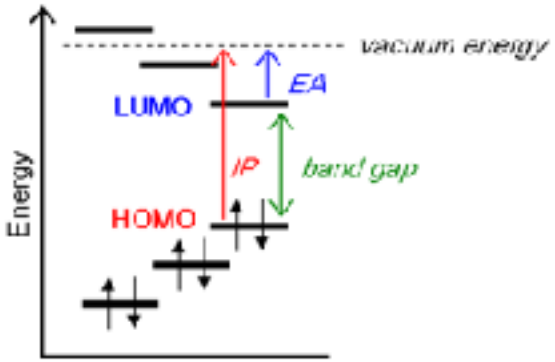
Qualitative Analysis of Electron Distribution

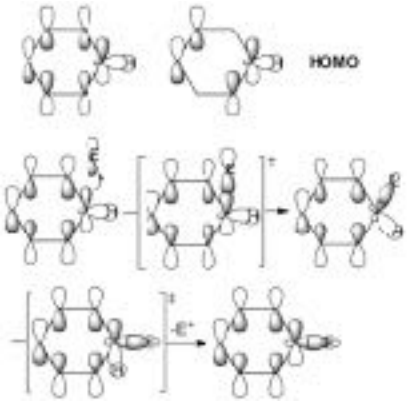


<= Polyene cyclization

Photocatalysis =>

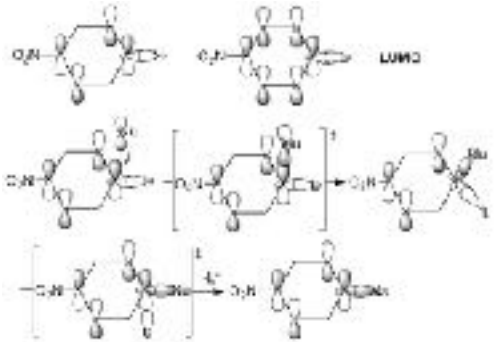






<= Electrophilic substitution

Nucleophilic substitution =>



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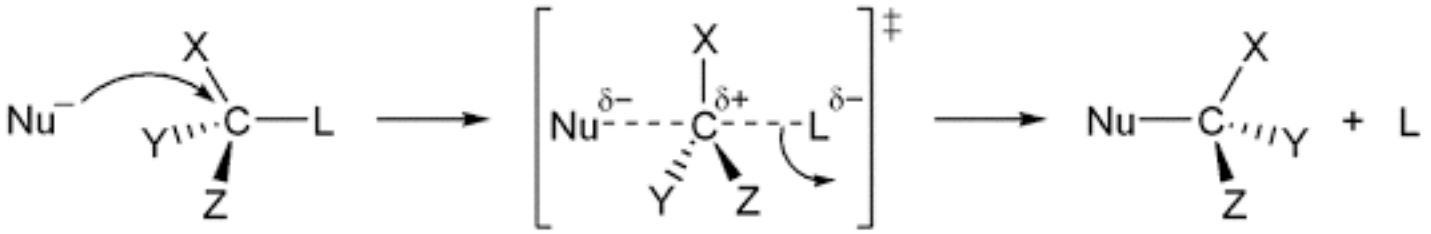
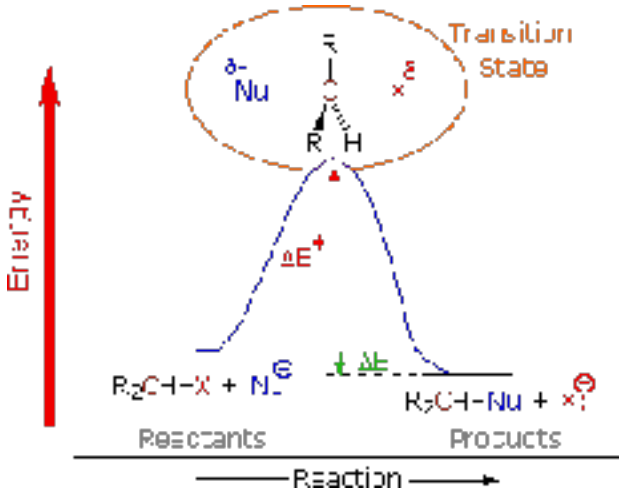
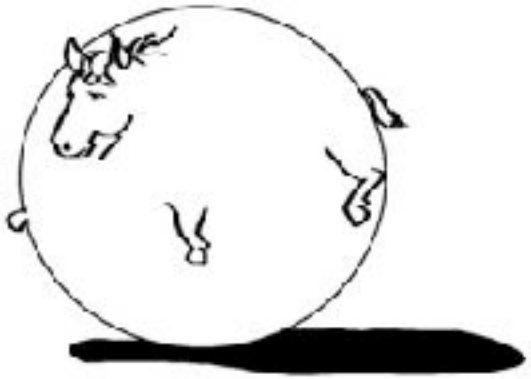
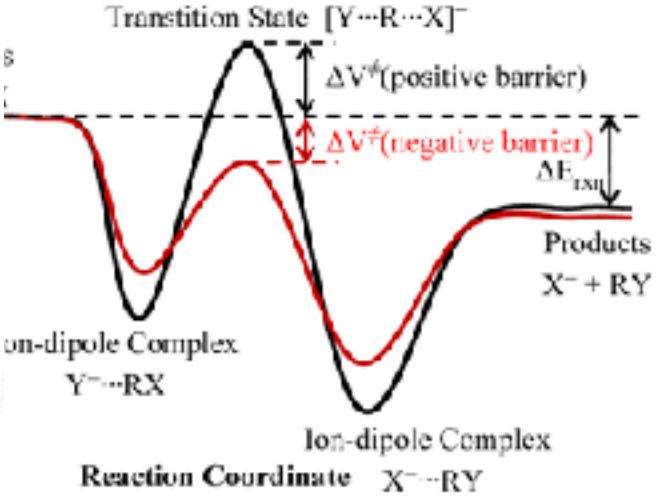
Theory vs Experiment: SN2 Reaction









Experiment

Solution
vs
Gas phase

Theory

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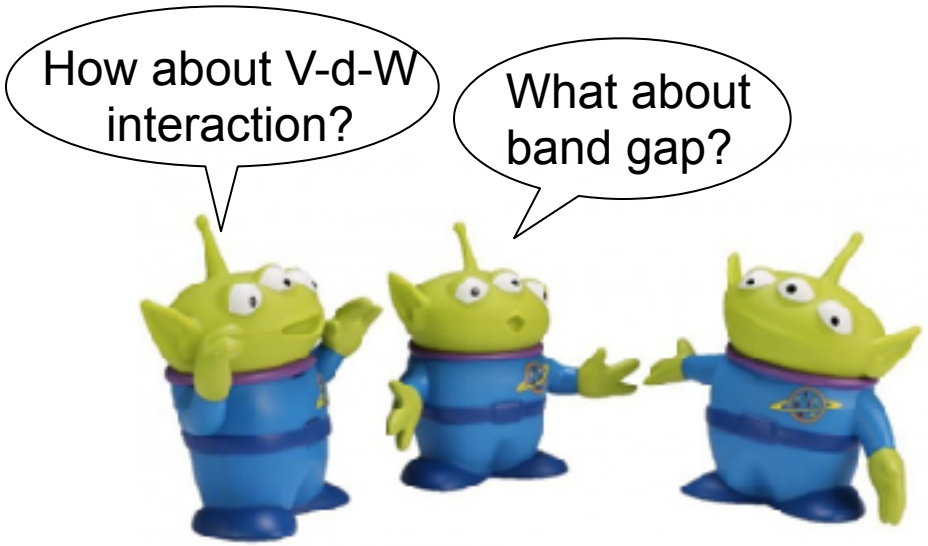
DFT Theory: Many flavors of potentials



$$V_{\mathrm{s}}(\vec{r}) = V(\vec{r}) + \int \frac{e^2 n_{\mathrm{s}}\left(\vec{r}'\right)}{\left|\vec{r} - \vec{r}'\right|} \mathrm{d}^3 r' + V_{\mathrm{XC}}[n_{\mathrm{s}}(\vec{r})]$$

$$E_{\mathrm{xc}}^{\mathrm{B3LYP}} = E_{\mathrm{x}}^{\mathrm{LDA}} + a_0(E_{\mathrm{x}}^{\mathrm{HF}} - E_{\mathrm{x}}^{\mathrm{LDA}}) + a_{\mathrm{x}}(E_{\mathrm{x}}^{\mathrm{GGA}} - E_{\mathrm{x}}^{\mathrm{LDA}}) + E_{\mathrm{c}}^{\mathrm{LDA}} + a_{\mathrm{c}}(E_{\mathrm{c}}^{\mathrm{GGA}} - E_{\mathrm{c}}^{\mathrm{LDA}}),$$

Thomas-Fermi (1927) => Honenberg-Kohn (1964) => TDDFT (1984) => LDA+GGA (1990s)

DFT Development: TDDFT

Runge-Gross theorem (1984): Analogue of Kohn-Sham theorem for TD

$$\left(-\frac{1}{2}\nabla^2 + v_s(\mathbf{r},t)\right)\phi_i(\mathbf{r},t) = i\frac{\partial}{\partial t}\phi_i(\mathbf{r},t) \quad \phi_i(\mathbf{r},0) = \phi_i(\mathbf{r}),$$

$$v_s(\mathbf{r},t) = v_{\text{ext}}(\mathbf{r},t) + v_J(\mathbf{r},t) + v_{\text{xc}}(\mathbf{r},t). \qquad \rho_s(\mathbf{r},t) = \sum_{i=1}^{N_\text{b}} f_i(t)|\phi_i(\mathbf{r},t)|^2,$$

Linear response TDFT

$$H'(t) = H + \delta V^{ext}(t) \qquad H'_{KS}[\rho](t) = H_{KS}[\rho] + \delta V_H[\rho](t) + \delta V_{xc}[\rho](t) + \delta V^{ext}(t)$$

$$\delta\rho(\mathbf{r}t) = \chi_{KS}(\mathbf{r}t, \mathbf{r}'t')\delta V^{eff}[\rho](\mathbf{r}'t')$$

Dyson equation

$$\chi(\mathbf{r}_1t_1, \mathbf{r}_2t_2) = \chi_{KS}(\mathbf{r}_1t_1, \mathbf{r}_2t_2) + \chi_{KS}(\mathbf{r}_1t_1, \mathbf{r}'_2t'_2)\left(\frac{1}{|\mathbf{r}'_2 - \mathbf{r}'_1|} + f_{xc}(\mathbf{r}'_2t'_2, \mathbf{r}'_1t'_1)\right)\chi(\mathbf{r}'_1t'_1, \mathbf{r}_2t_2)$$

Excitation energies are the poles of the linear response function

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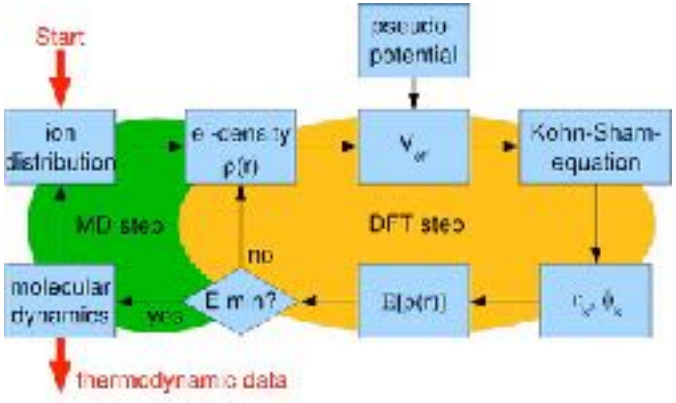
DFT Development: FT-KS-DFT



Molecular dynamics $m_I \ddot{\mathbf{R}}_I = -\vec{\nabla}_I V(\mathbf{R}_1, \mathbf{R}_2, \ldots, \mathbf{R}_N)$

Born-Oppenheimer energy surface: $V(\{\mathbf{R}\}) = \Omega(\{\mathbf{R}\}) + E_{ion\text{-}ion}(\{\mathbf{R}\})$

Current best practice uses Free Energy Density Functional Theory with one-electron Kohn-Sham orbitals

$\Omega[n] = F[n] + \int d\mathbf{r}\,(v_{ext}(\mathbf{r}) - \mu)\, n(\mathbf{r})$ -- Grand potential

$F[n] = F_s[n] + F_H[n] + F_{xc}[n]$ -- Free-energy functional

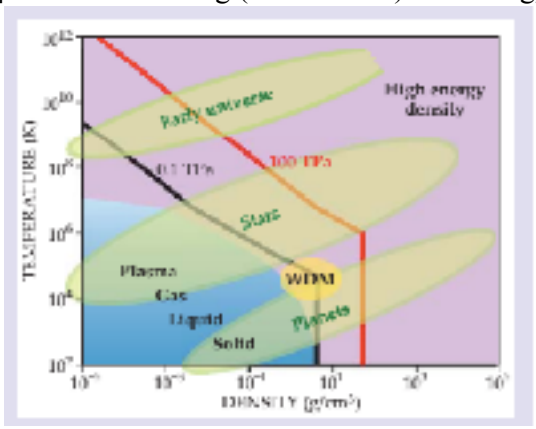
$F_H[n]$ -- Hartree energy

$F_{xc}[n]$ -- Exchange-Correlation (XC) free-energy

$F_s[n]$ -- Non-interacting (Kohn-Sham) free-energy

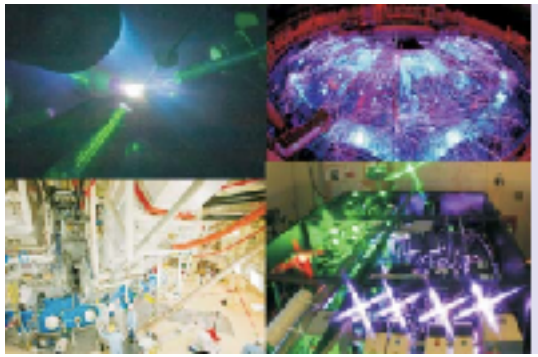
$$\left\{-\tfrac{1}{2}\nabla^2 + v_H(\mathbf{r};\{\mathbf{R}\}) + v_{xc}(\mathbf{r};\{\mathbf{R}\}) + v_{ext}(\mathbf{r};\{\mathbf{R}\})\right\}\varphi_j(\mathbf{r};\{\mathbf{R}\}) = \varepsilon_j\,\varphi_j(\mathbf{r};\{\mathbf{R}\})$$

$$n(\mathbf{r};\{\mathbf{R}\}) = \sum_j f(\varepsilon_j;\beta)\left|\varphi_j(\mathbf{r};\{\mathbf{R}\})\right|^2 \quad ; \quad v_{xc}[n] = \frac{\delta F_{xc}}{\delta n} \quad ; \quad \beta = 1/k_B T$$



Material properties

- Thermal conductivity;
- Absorption coefficients
- Electrical conductivity;
- Reflectivity



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R.P. Drake, Physics Today, June 2010, 28-33

DFT Applications to solid state materials

Two most popular solid-state DFT codes

VASP

b-initio VASP ackage ienna imulation

Plane waves

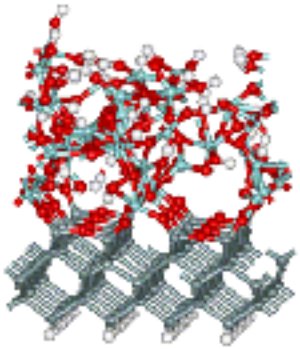
SIESTA

siesta

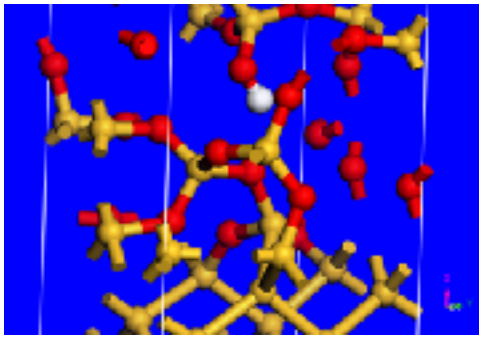
Localized orbitals

Interplay of quantum chemistry and solid state theory applications

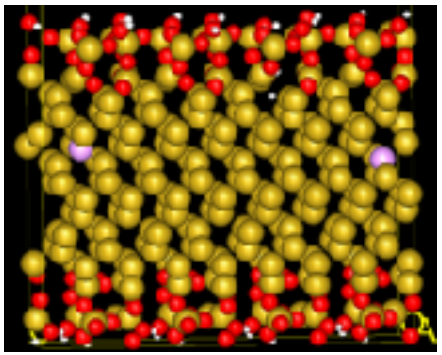
Deposition



Defect formation



Device design



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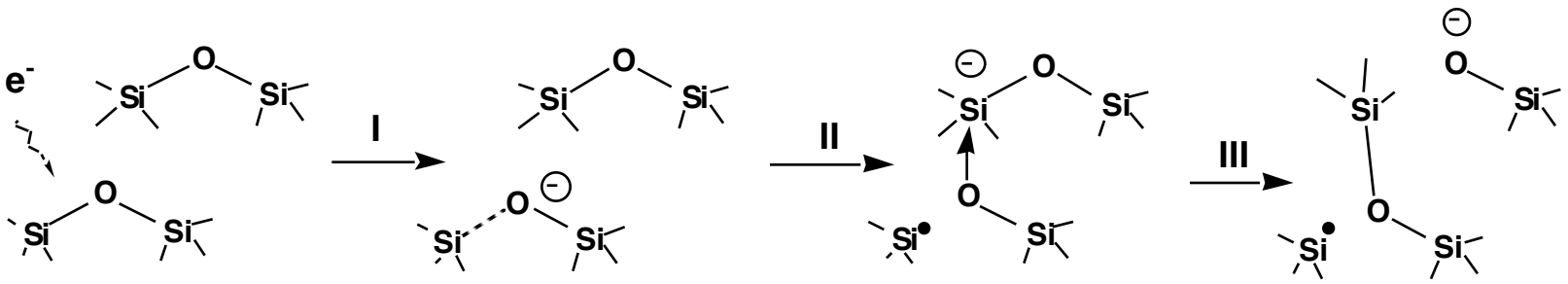
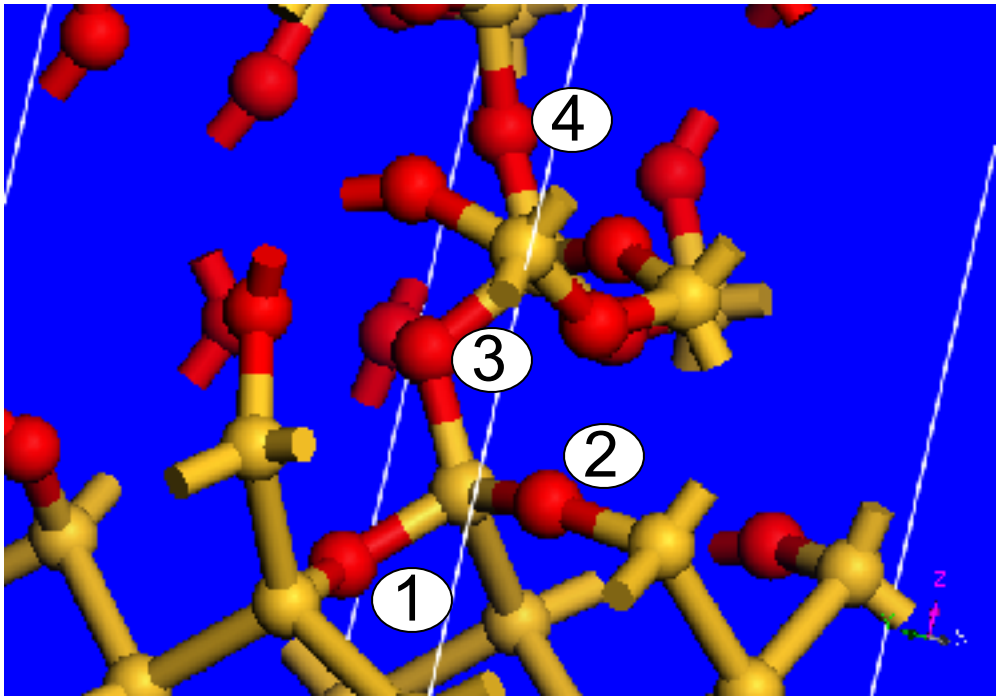
Defect generation at Si/SiO_2 interface





E in EV:

O4 = 0.39

O3 = 0.55

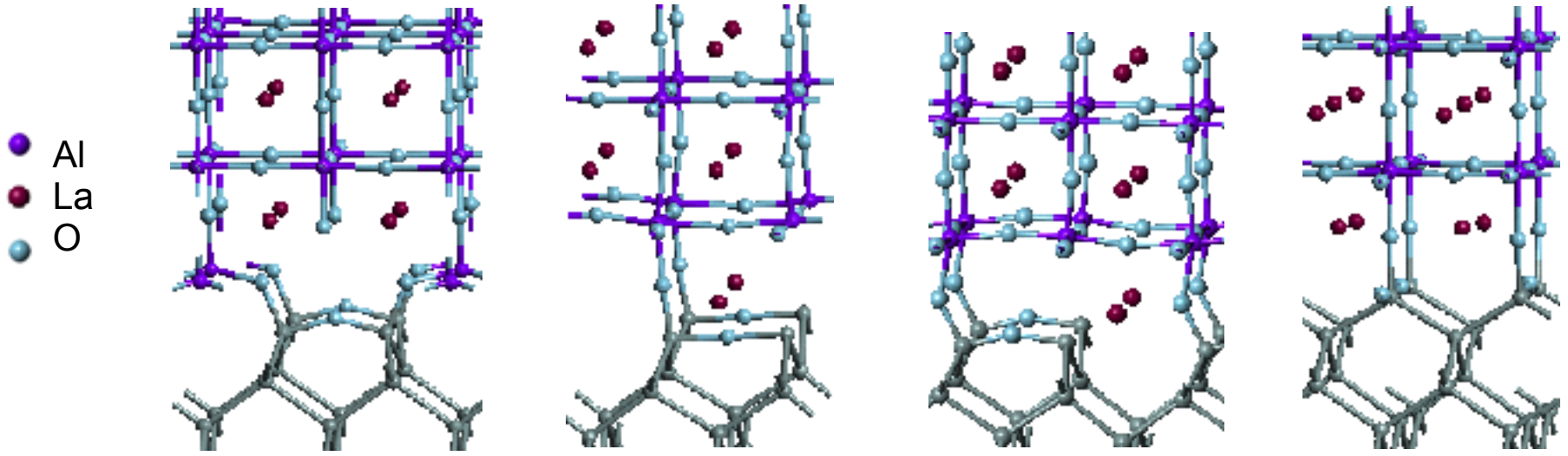
O2 = 0.27

O1 = 0.0

Bersuker, G.; Korkin, A.; et al., Microelectronic Engineering, 2003, 118-129.

Modeling of $LaAlO_3$/Si Interface

№ 1 AlO2-term.	№ 2(intra) LaO-term.	№ 2(inter) LaO-term.	№ 3 O-shifted

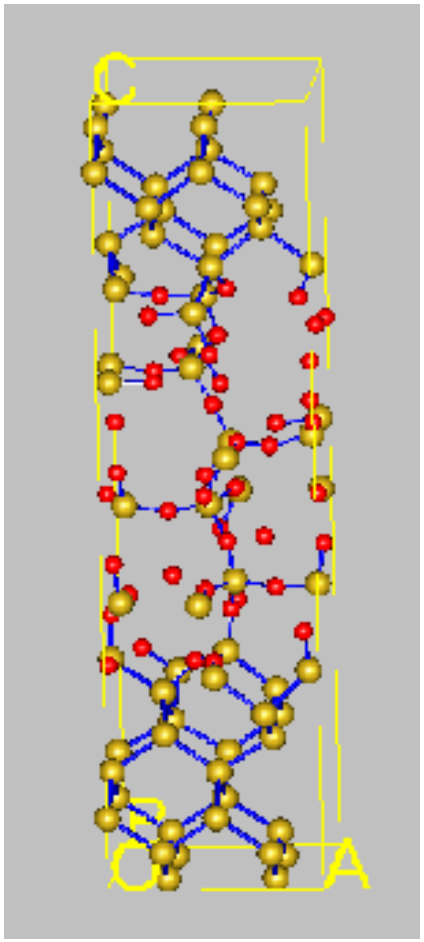


2x1 Si(001)	2x1 Si(001)	2x1 Si(001)	2x2 Si(001)

Relative energy	+4.8 eV	+ 0.8 eV	+0.0 eV	0.0 eV

Knizhnik, A.A.; Iskandarova И.; Bagaturyants, A.; Potapkin, Б.В.; Fonseca, L.R.C.; Korkin A. Phys. Rev.B. 2005, 72, 235329.

Modeling of $Si/SiO_2/Si$ Interfaces



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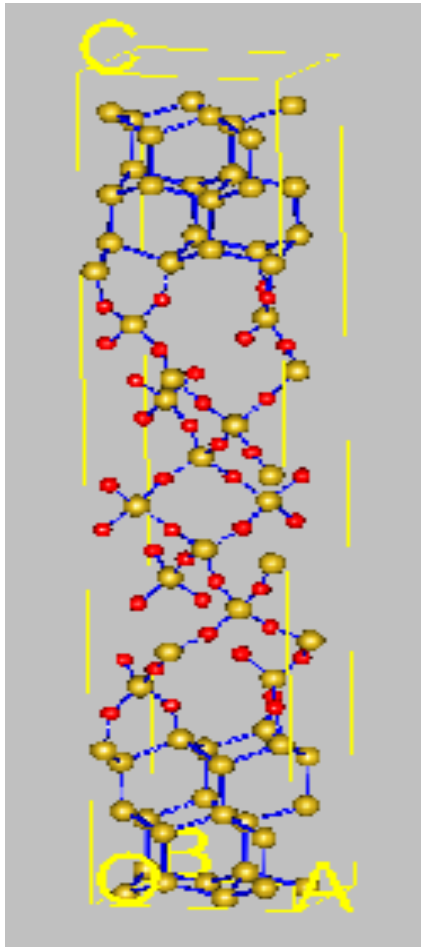

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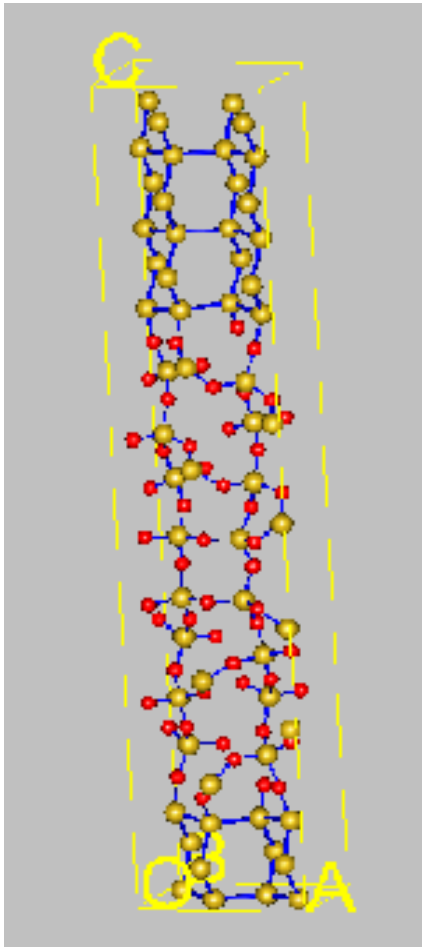


(110)

Korkin, A.A.; Greer, J.; Bersuker, G.; Karasiev, V.; Bartlett, R.J.
Phys. Rev. B. 2006, 73, 165312.

$ZrSiO_4$ Polymorphs

Why do we care about $ZrSiO_4$ polymorphism?

Electronics: Potential high-k material. Various nanocrystalline forms or different bonding patterns may exist in deposited thin films

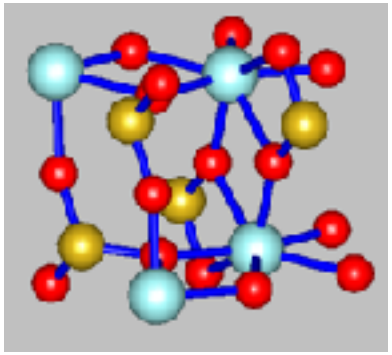
Nuclear safety: Zircon is used to preserve nucleotides imbedded in its lattice. Defects and radioactive damage may modify the structure

Geochemistry: Computational design help to discover new minerals and study the earth history and resources.

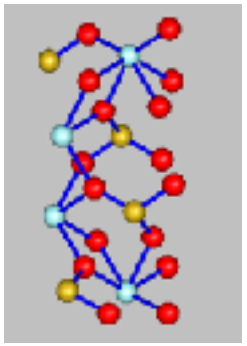
What is known about $ZrSiO_4$ polymorphism?

Zircon:

Stable form



Tetragonal
$I4_1/a$
Z=4
ABO



Reidite:

High pressure

Korkin, A.A.; Kamisaka, H.; Yamashita, K.; Safonov, A.; Bagatur'yants, Appl. Phys. Lett. 2006, 88, 181913.

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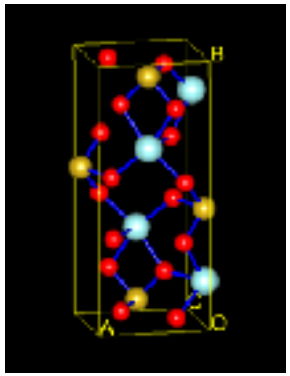
High density crystal structures

Zr/Si:

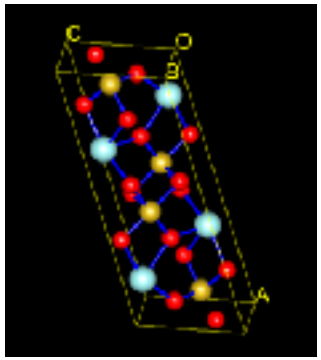
6/6:

Alumotantite ($AlTaO_4$)



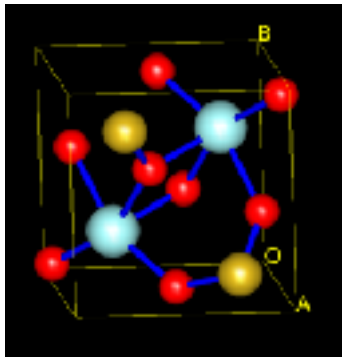
Orthorombic
E=0.78 eV; d=4.95

Raspite ($PbWO_4$)



Monoclinic
E=0.79; d=5.03

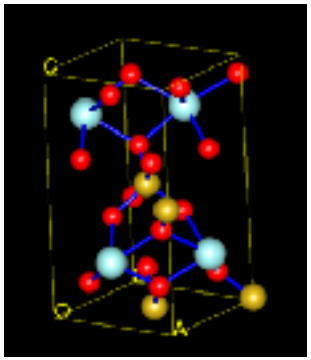
Wolframite ($MnWO_4$)



Monoclinic
E=1.06; d=5.28

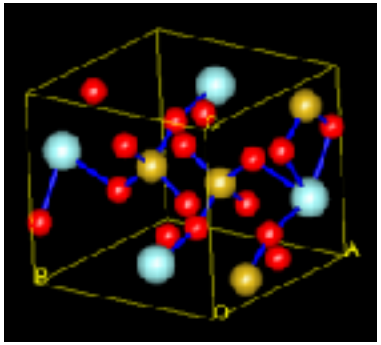
8/4:

Stibiocolumbite ($SbNbO_4$)



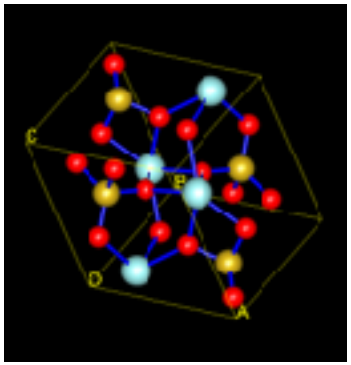
Orthorombic
E=0.72; d=5.18

Anhydrite ($CaSO_4$)



Monoclinic
E=0.74; d=4.66

Monazite ($EuPO_4$)



Monoclinic
E=1.04; d=4.91

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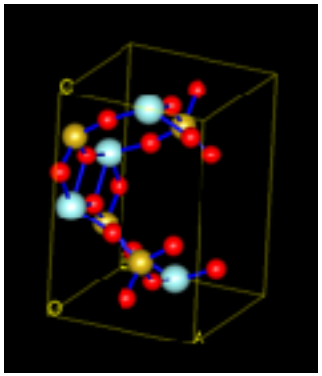
Low density crystal structures

Zr/Si:

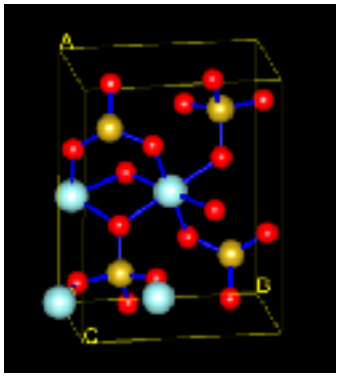
6/4:

Anhydrite ($CaSO_4$)



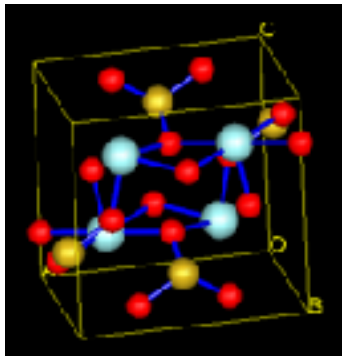
Orthorombic
E=0.49 eV; d=3.23

Chalcocyanite ($CuSO_4$)



Orthorombic
E=0.96; d=4.06

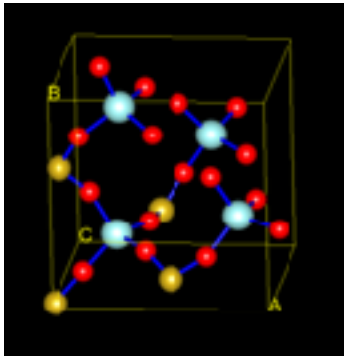
Barite ($BaSO_4$)



Orthorombic
E=1.25; d=4.52

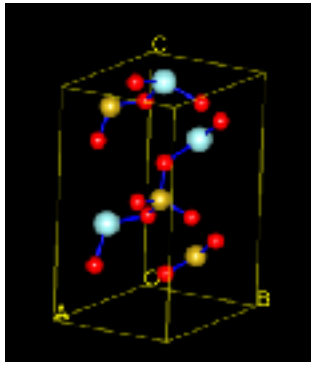
4/4:

β-Crystobalite (SiO_2)



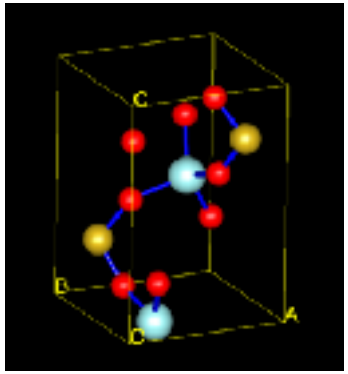
Cubic
E=0.94; d=2.40

Rodolicoite ($FePO_4$)



Hexagonal
E=1.25; d=3.13

Crystobalite (SiO_2)



tetragonal
E=1.32; d=2.75

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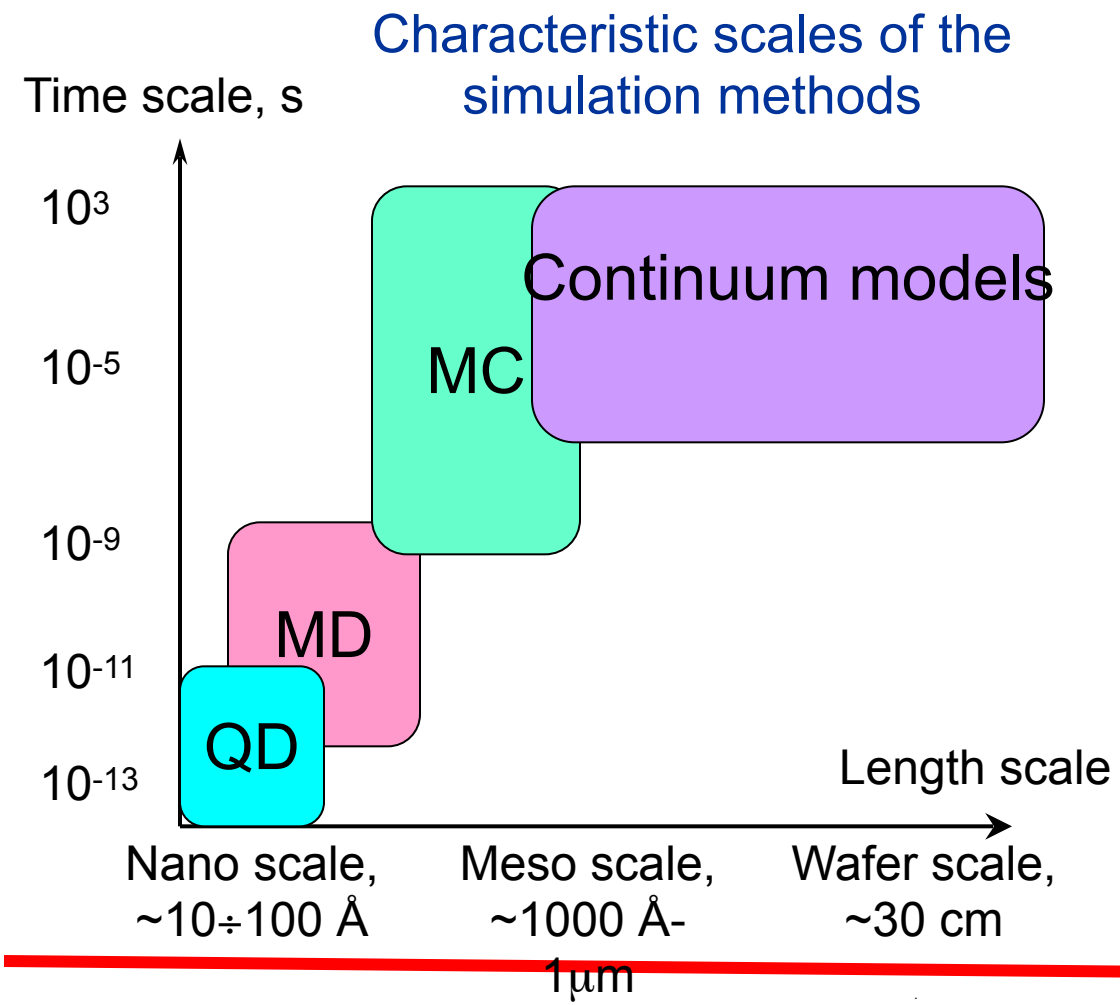
Size & Time Scale Limits of Different Models



QD- quantum dynamics

MD molecular dynamics, based on (semi-)empirical potentials

MC - kinetic Monte Carlo models, including lattice kMC

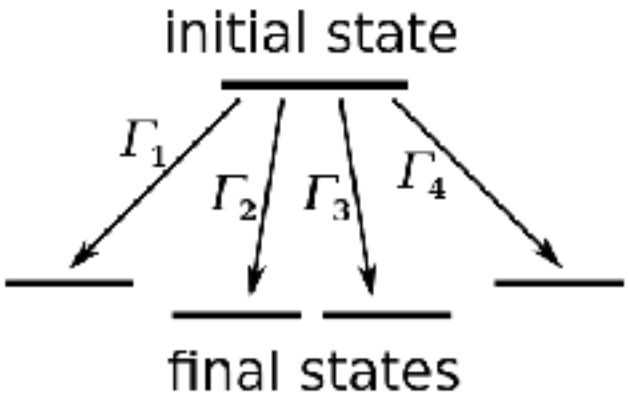
Monte Carlo Simulation

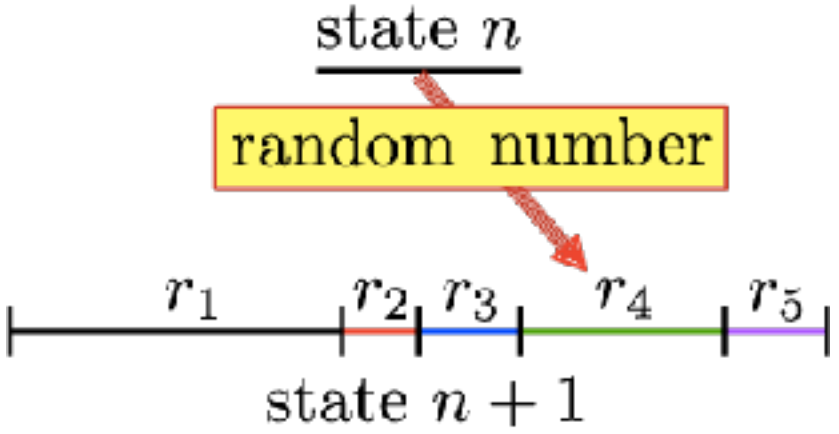
General idea => Considering a statistically representative part
of the system instead of the whole system to study any given property

Metropolis algorithm

Energy minimization and calculation of average properties => accepting structures with lower energy than starting point (P = 1) and higher energy (P = exp [- (E2-E1)/kT]

Kinetic Monte Carlo





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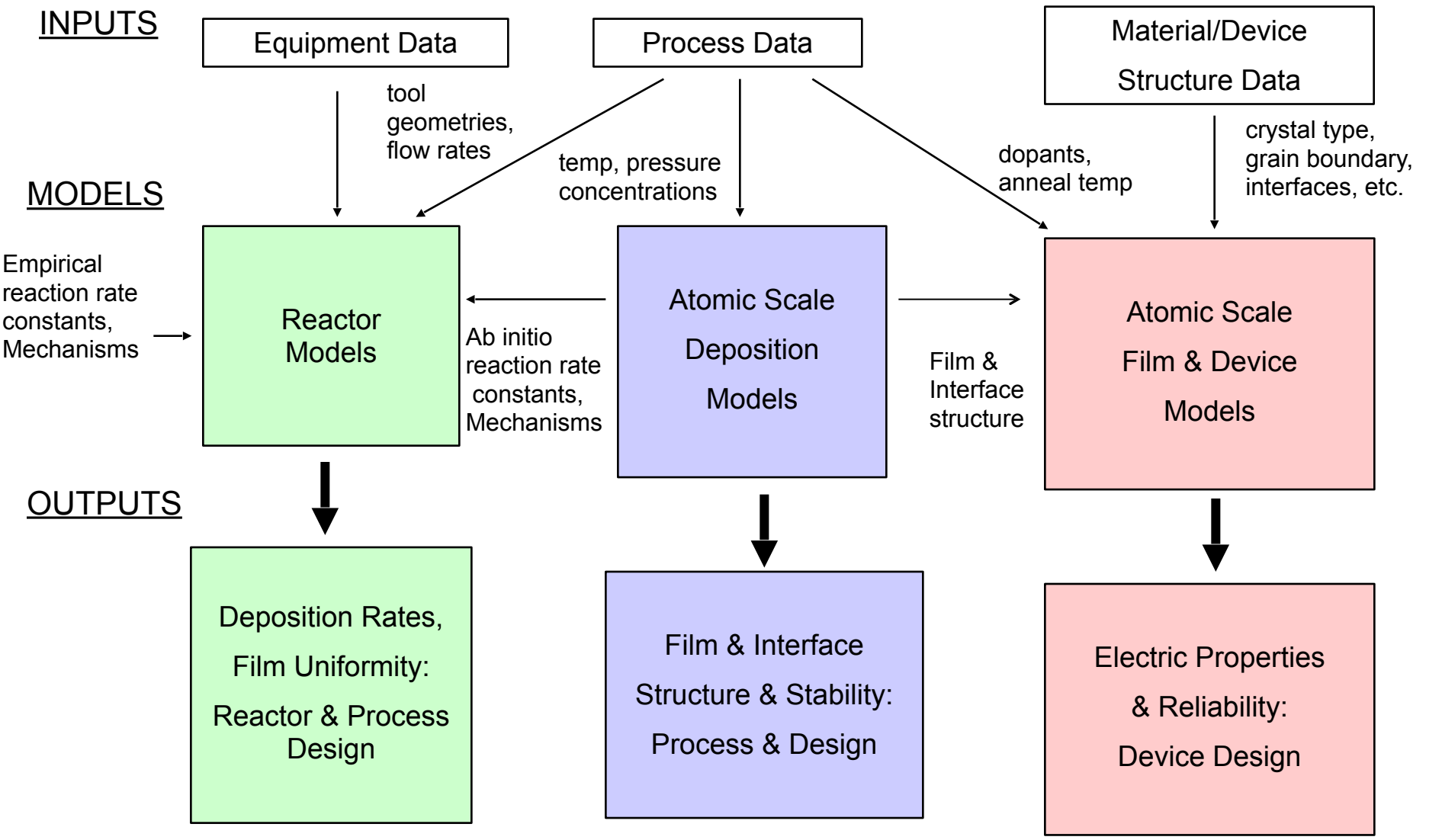
Computational materials and devices at electronic industry



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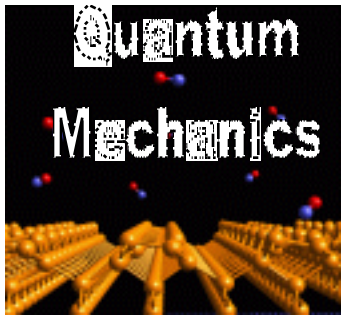
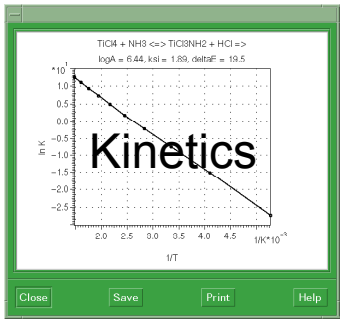
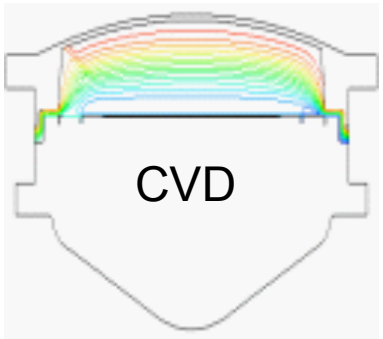
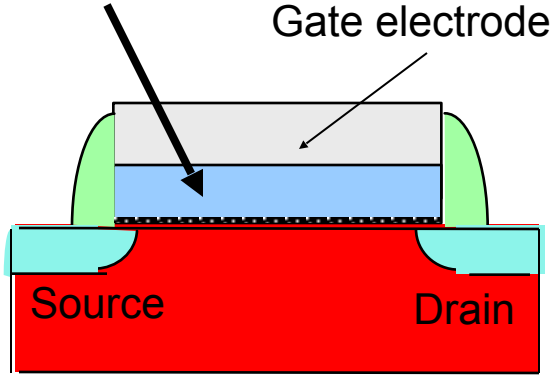
High-K dielectrics: from deposition to the film structure and properties

New Gate Oxide ?









Multi-scale + Multi-skills

Process ↔ Material
Material ↔ Device

CVD ↔ Å-scale ↔ I-V

Process ↔ Device

Metal Oxides

- \+ *Permittivity*
- ? *Band gap*
- ? *Band offset*
- ? *Charge traps*
- ? *Processability*
- ? *Stability*
- ? *Reliability*
- ? …

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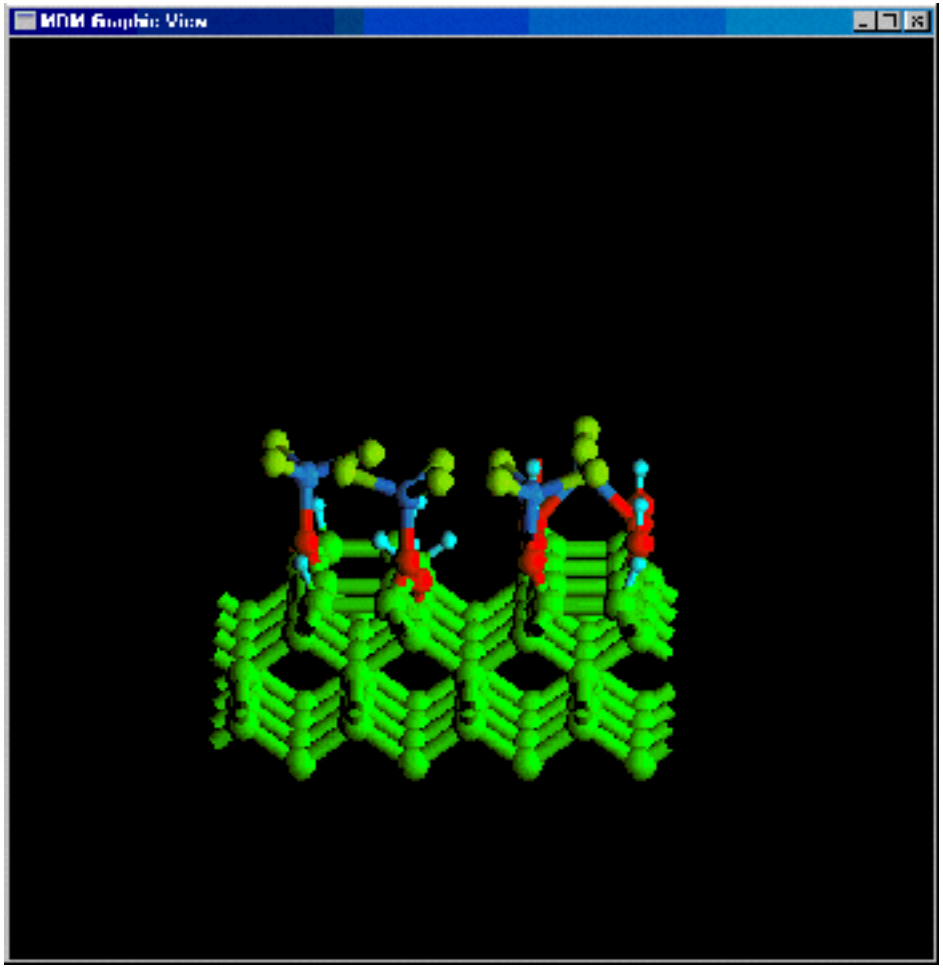
An Integrated kMC-MD approach: ZrO_2 ALD Modleing

DFT cluster & periodic study:
reacting molecules and barriers

Chemical kinetics calculations:
elementary chemical reactions

Molecular dynamic simulation:
conformations & surface relaxation

Kinetic Monte Carlo simulation:
interface formation & film growth



A snapshot of an interface formation

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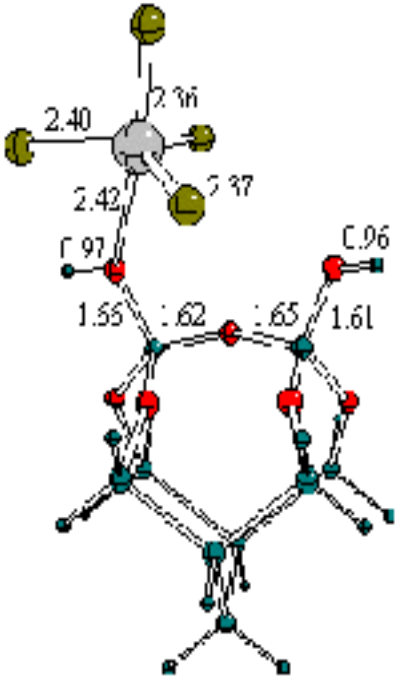
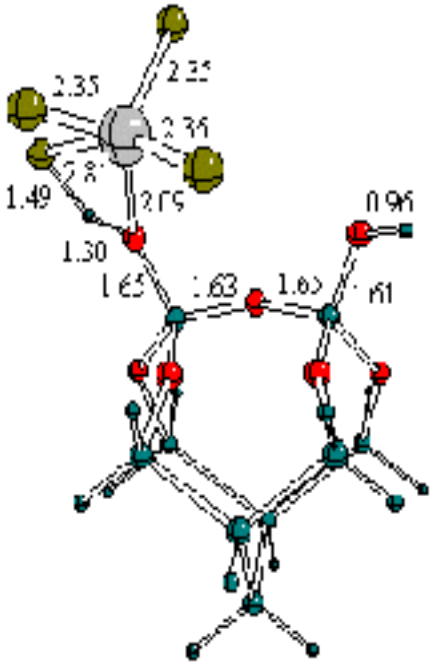
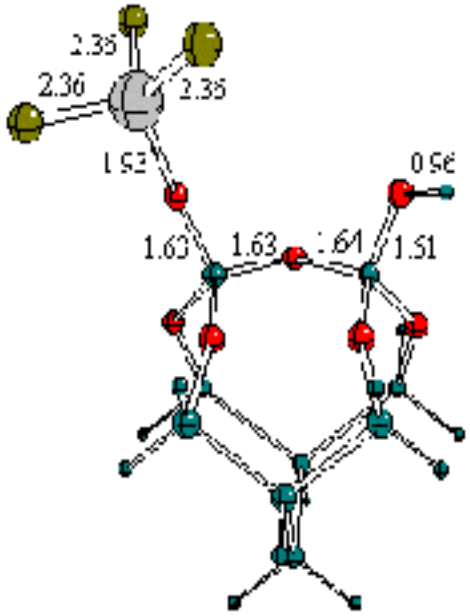
$ZrCl_4$ Adsorption on OH Terminated Si(100) Surface



I



II



III

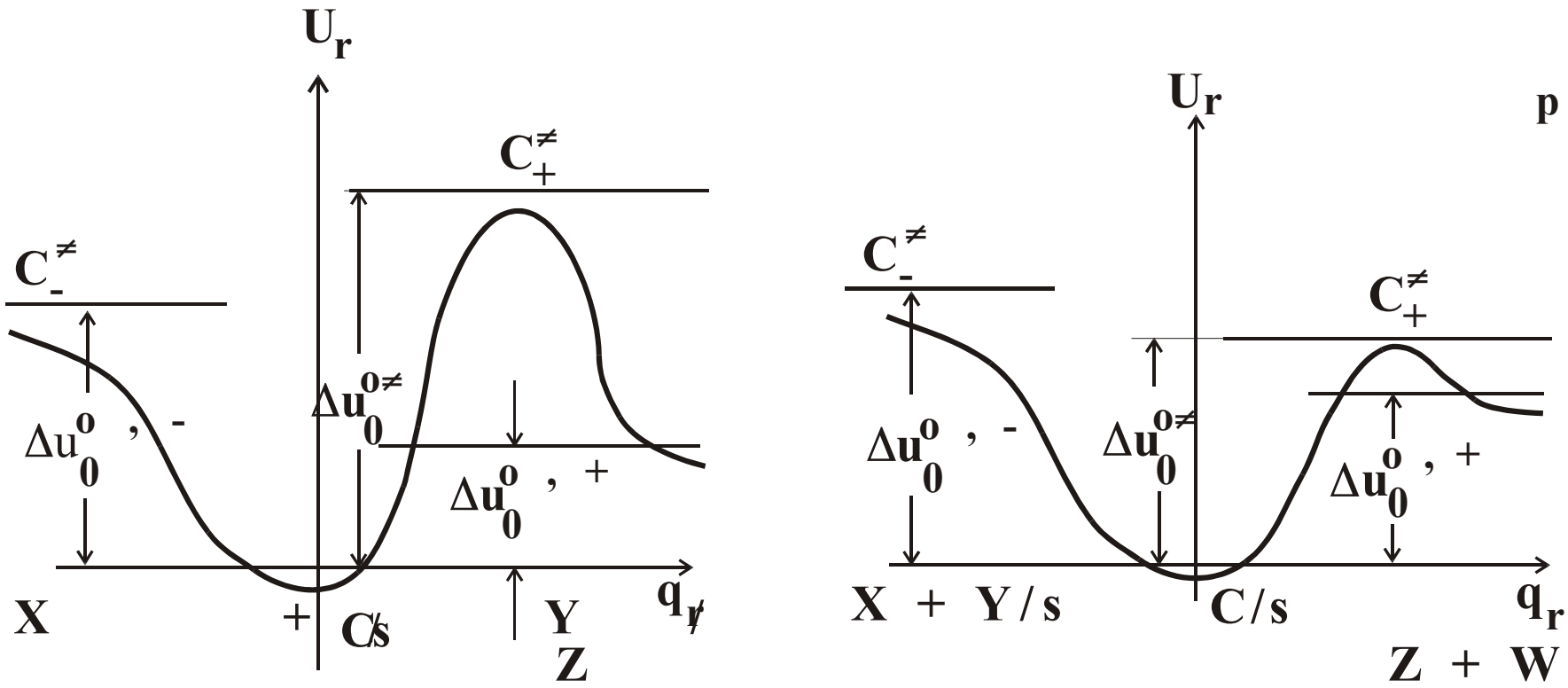
	Adsorption complex	Transition state	Product
ΔE (in kcal/mol)	-12.1	+1.7	-5.2

Kinetics of Gas-Surface Reactions

- REACTION PATH PROFILES

  $X + Y/s \Longrightarrow Z + W/s$

- $X=MCl_4$; $Y/s=\{Si\}–OH$; $Z = HCl$; $W/s = \{Si\}–OMCl_3$; $M = Zr, Hf$



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Lattice kMC Model of Zirconia Film Growth

First ALD step

- $ZrO(s) + H2O(g) \Rightarrow Zr(OH)2(s)$
- $ZrCl(s) + H2O(g) \Rightarrow Zr(OH)(s) + HCl(g)$
- $ZrOZrCl3(s) + Zr(OH)(s) \Rightarrow (ZrO)2ZrCl2(s) + HCl(g)$

Diffusion processes

- $O + v \Rightarrow v + O$
- $OH + O \Rightarrow O + OH$
- $Cl + v \Rightarrow v + Cl$

Second ALD step

- $Zr(OH)(s) + ZrCl4(g) \Rightarrow ZrOZrCl3(s) + HCl(g)$
- $2Zr(OH)(s) + ZrCl4(g) \Rightarrow (ZrO)2ZrCl2(s) + 2HCl(g)$
- $3Zr(OH)(s) + ZrCl4(g) \Rightarrow (ZrO)3ZrCl(s) + 3HCl(g)$
- $ZrOZrCl3(s) + Zr(OH)(s) \Rightarrow (ZrO)2ZrCl2(s) + HCl(g)$

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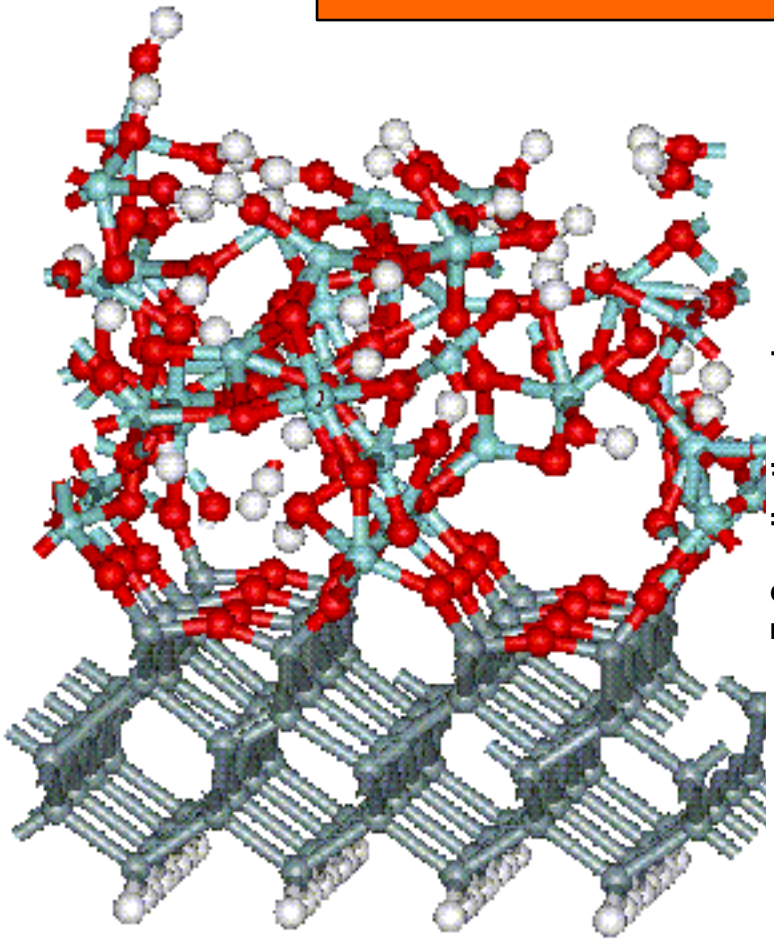
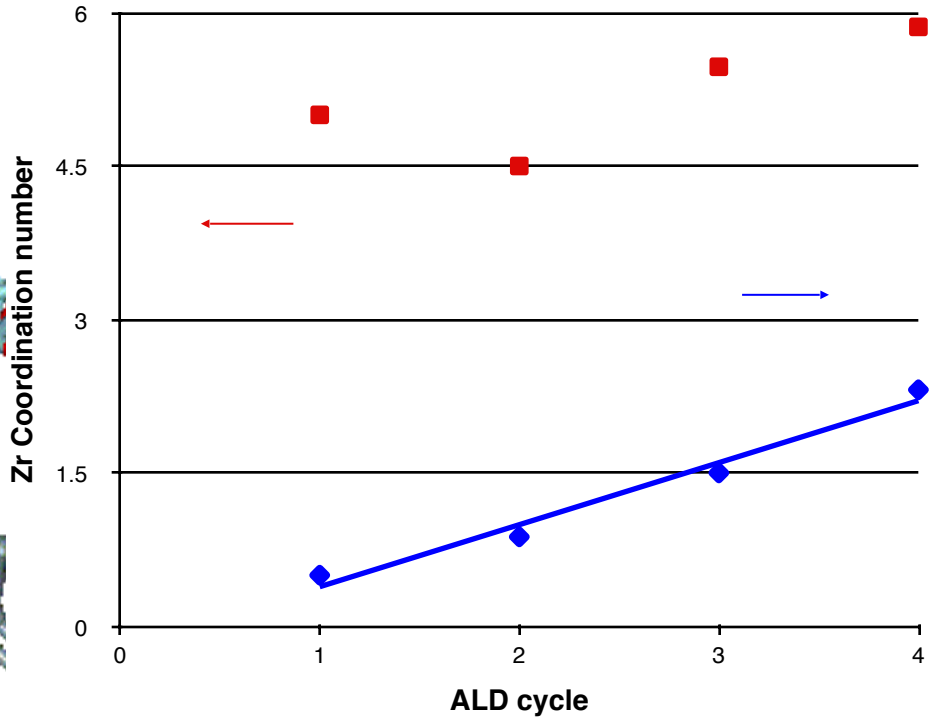
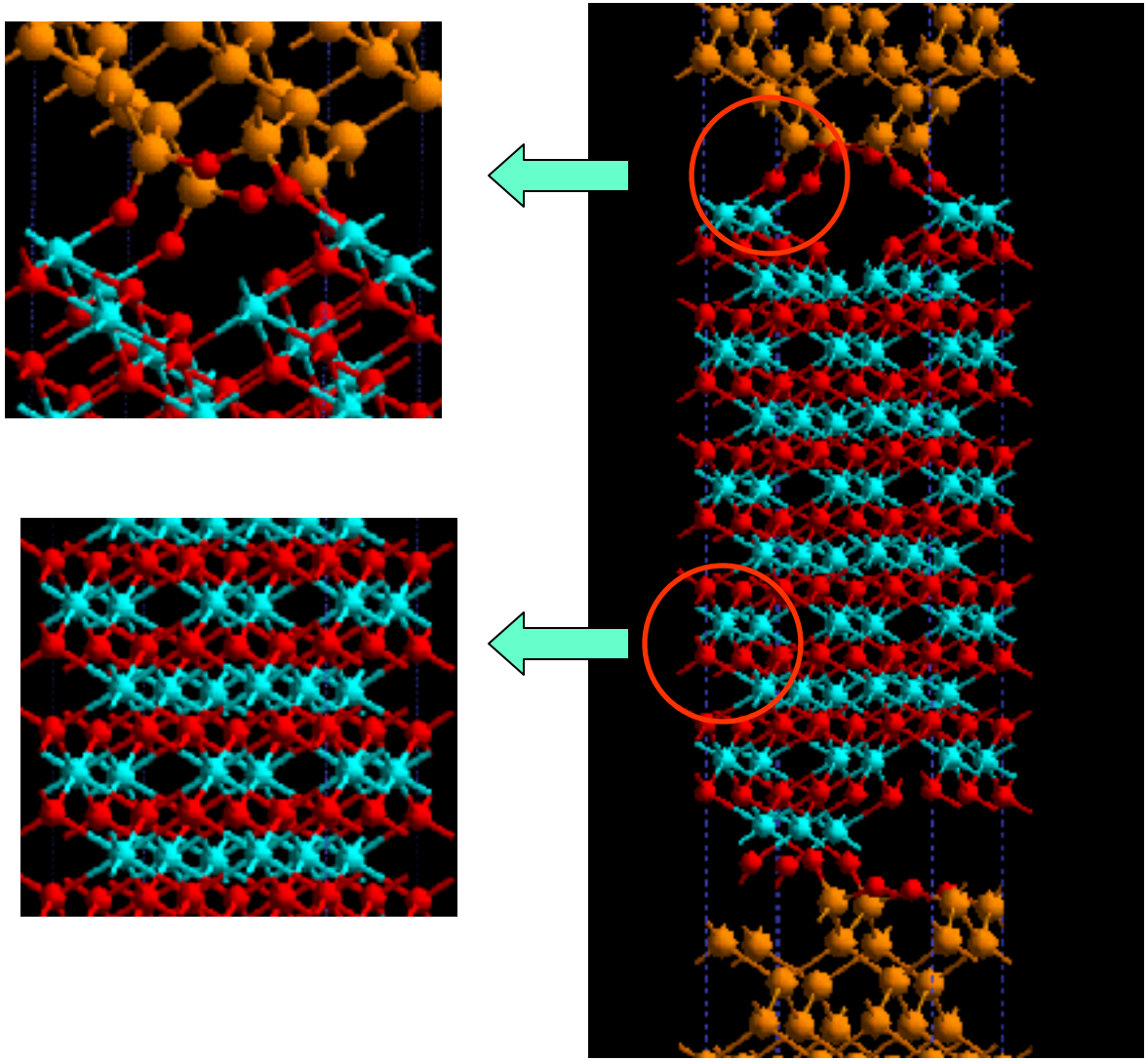
$ZrCl_4 + H_2O$ ALD: Low density of the first layers



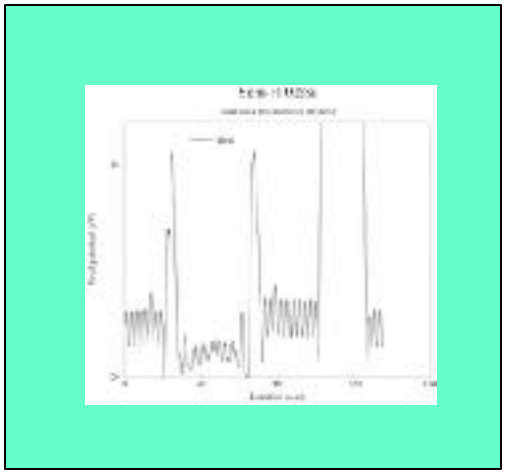


Deminsky, M.; Knizhnik, A.; Belov, I.; Umanskii, S.; Rykova, E.; Bagatur'yants, A.; Potapkin, B.; Stoker, M.; Korkin, A. Surface Science, 2004, 549, 67-86.

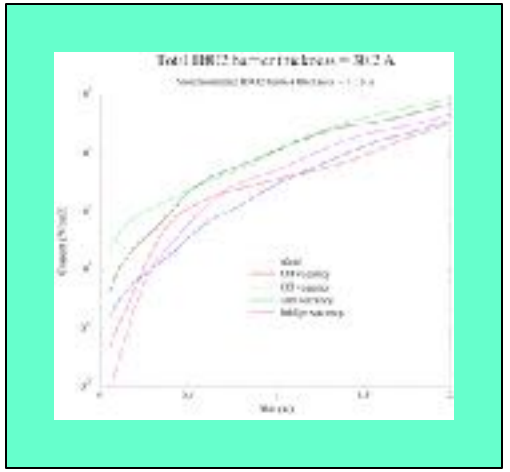
$Si/ZrO_2/Si$ Gate Stack Model



Total potential (eV)



Leakage current (A/cm^2)



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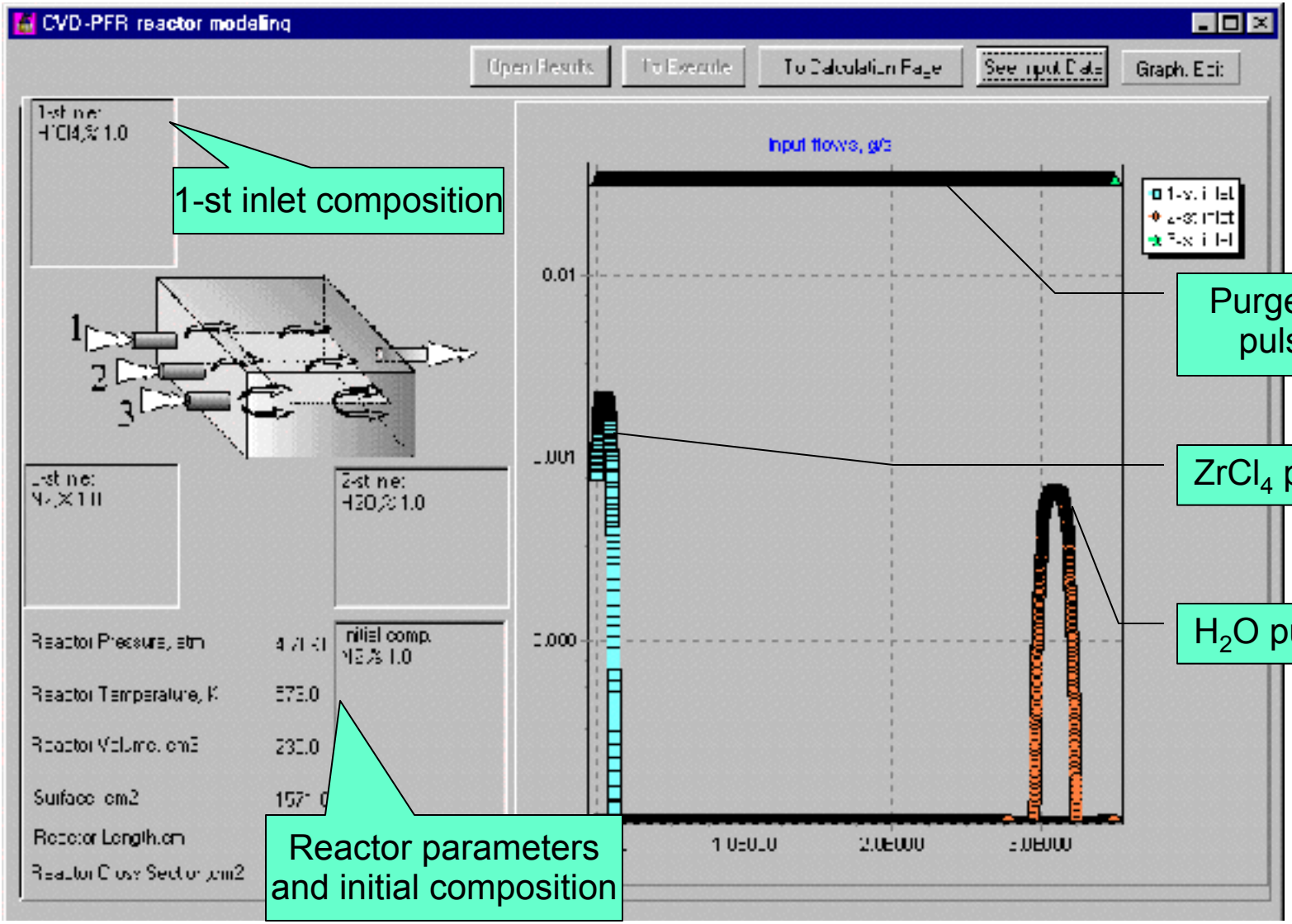
Plug Flow Reactor Model



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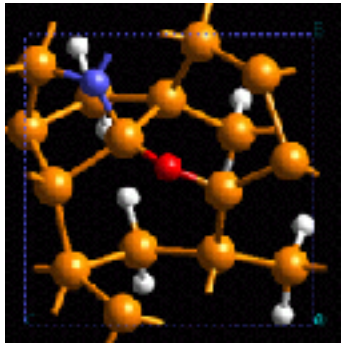
KHIMERA: Kinetics from Molecules to Reactor

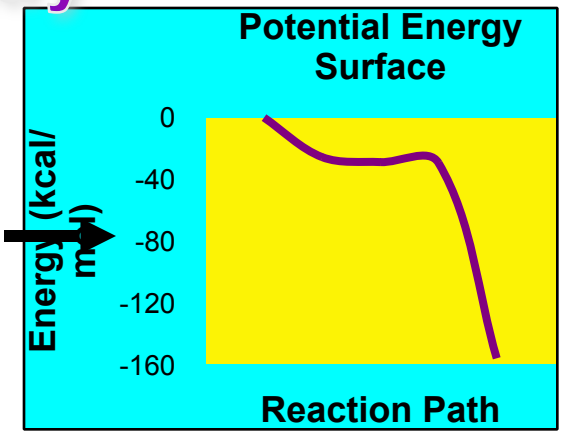
I. Quantum chemistry

Reactant

Transition state



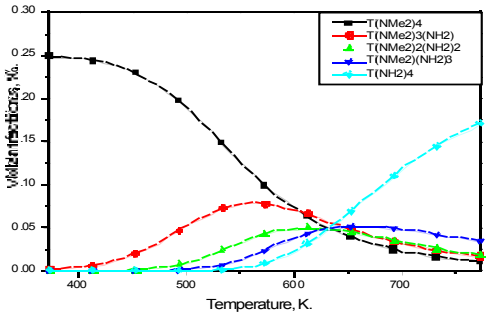
Product



Minimum energy path

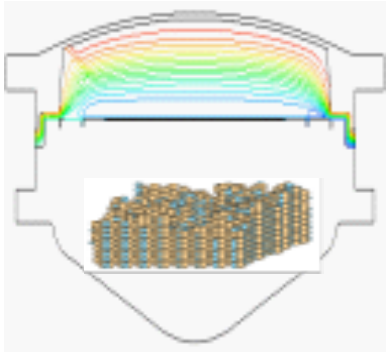
II. Chemical Kinetics

Individual reaction rates



Complex chemical kinetics

III. Reactor Modeling



Chemistry in CVD reactor

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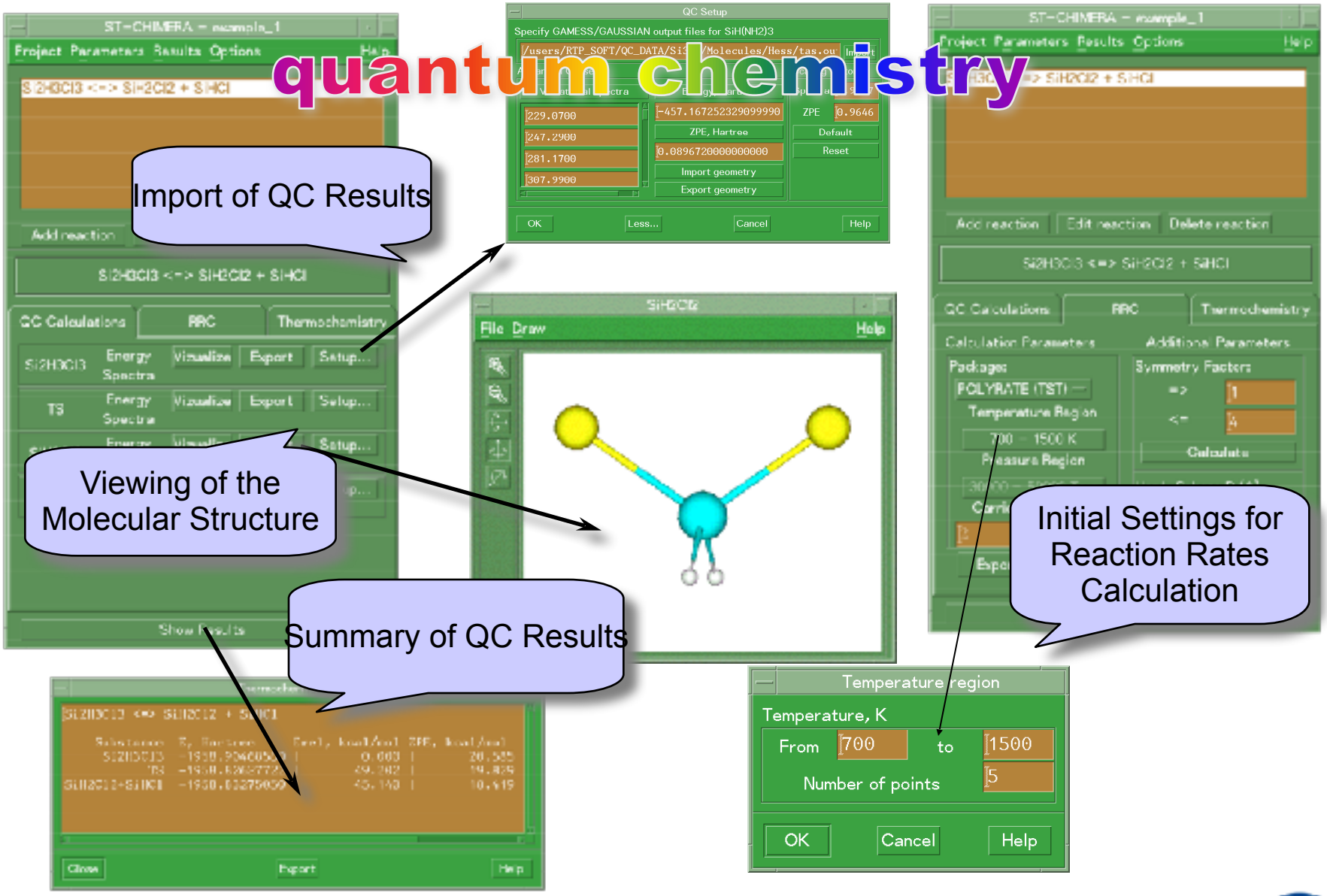
quantum chemistry



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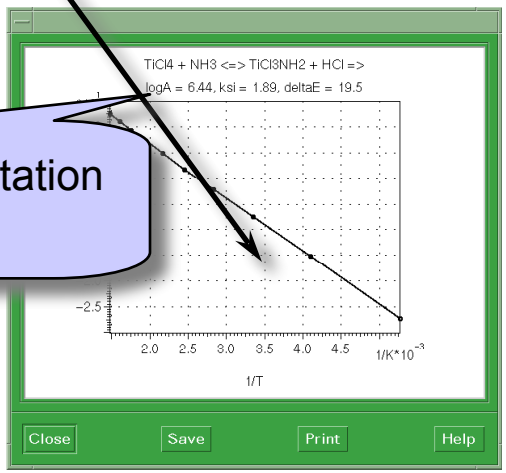
Calculated Reaction Rates

Individual rate constants

Results of Thermochemical Calculations

Graphical Representation of Results



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Reactor modeling

Model, and process conditions

Reactor parameters | Calculation parameters

Reactor type: Well-Stirred

T = 973 K

P = 50 Torr

V = 840 sm**3

Carrier gas: N2

OK

Initial conditions and calculation details

Reactor parameters | Calculation parameters

Calculation type: C(t)

Solving method: Explicit

Residence time 5 s

Time step 0.001 s

Initial conditions:

N2	7000	sccm
ACS	0	sccm
ADCS	0	sccm
DCS	30	sccm

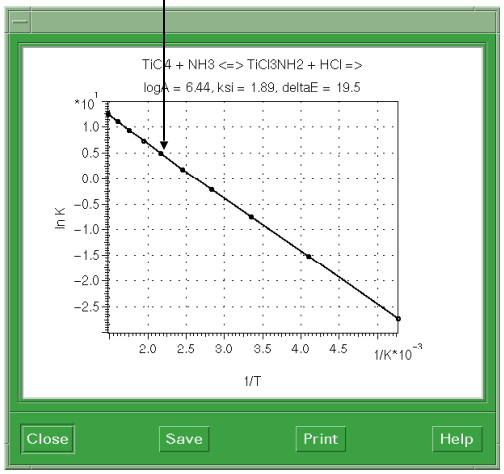
OK | Cancel | Help

Results

Reactor results

- H2
- NH3
- SiCl2
- SiH2Cl2
- SiH2NH2Cl
- SiHCl
- SiHNH2Cl2

Show | Close | Help



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Cheminformatics: Application of Data Science in Chemistry and Materials Science

Term introduced by F.K. Brown in 1998

Basic paradigm

Quantum chemistry => wave/particle dualism
Molecular mechanics => atomic structure of matter
Cheminformatics => chemical space

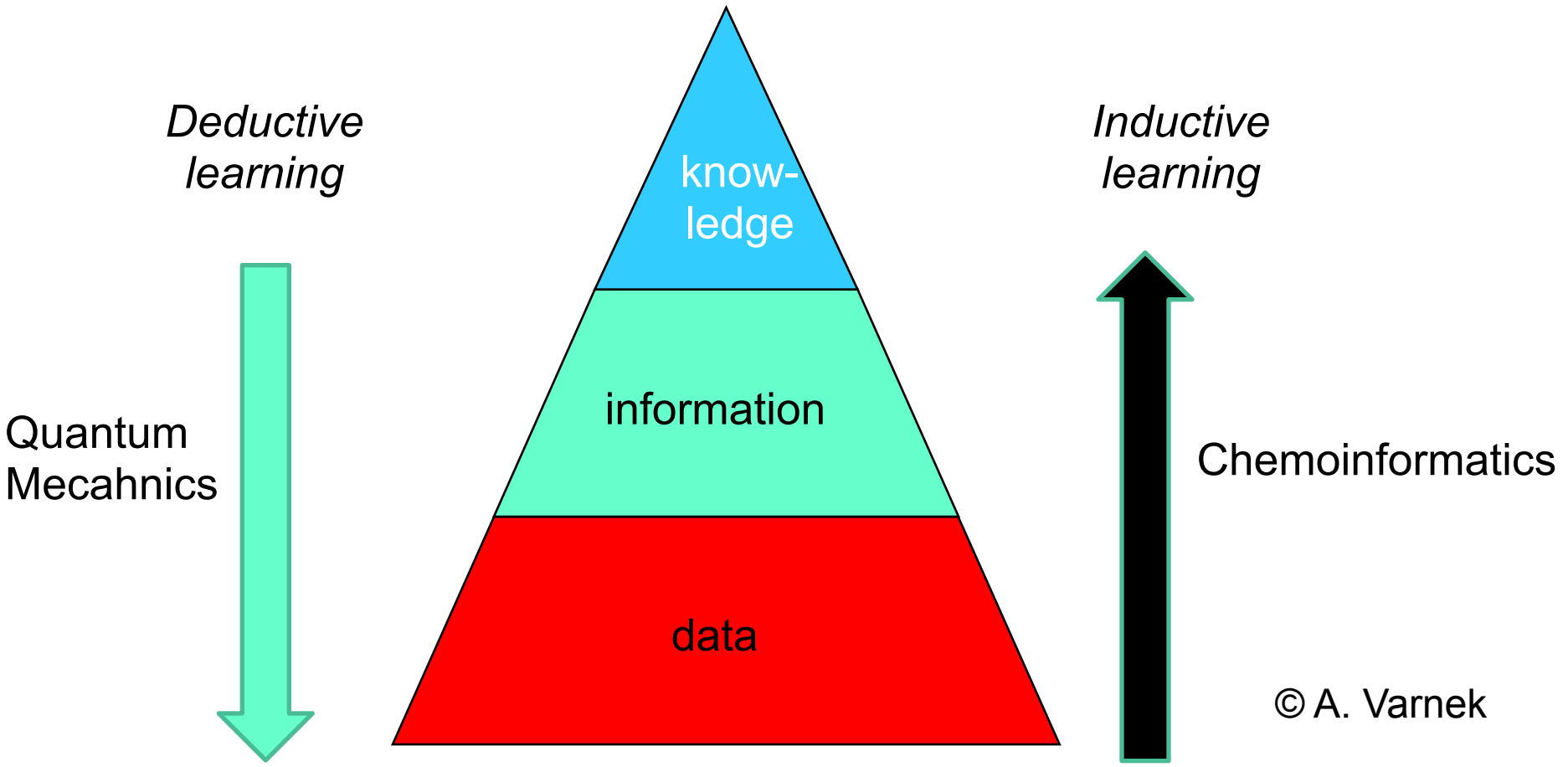
Basic model

Quantum chemistry => electron and nuclei
Molecular mechanics = > atoms and bonds
Chemoinformatics => molecular graph and decsriptor vectors

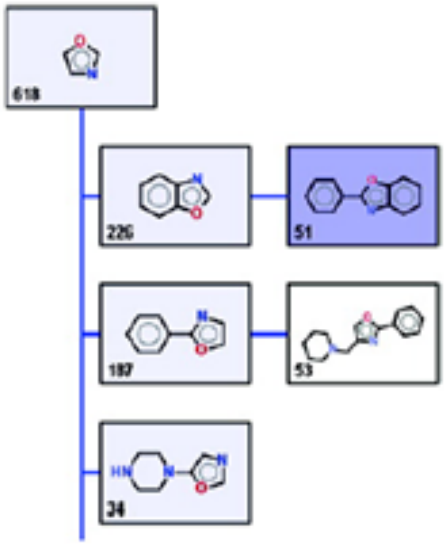
Basic theory

Quantum chemistry => Schroedinger equation
Molecular mechanics => classical and statistics mechanics
Cheminformatics => graph theory and statistics based learing

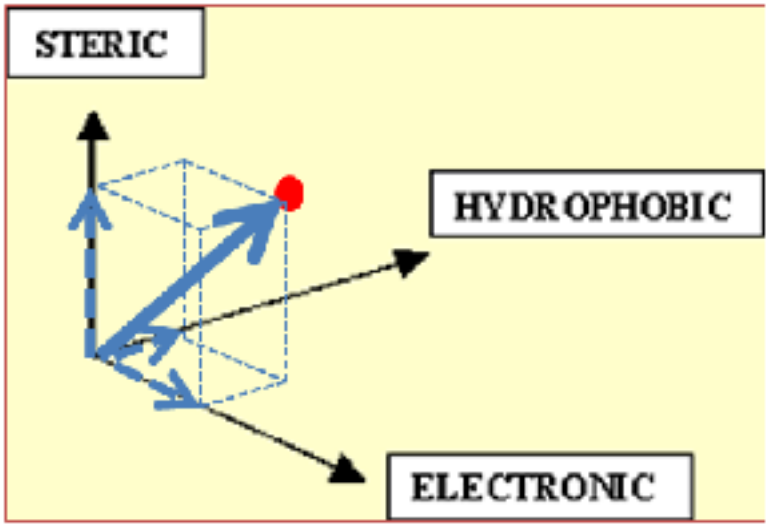
Cheminformatics: from Data to Knowledge



Chemical Space Paradigm



graphs-based



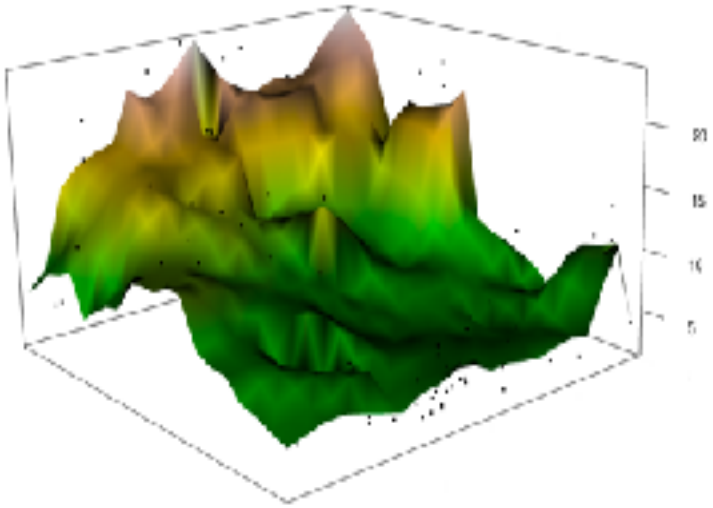
descriptors -based

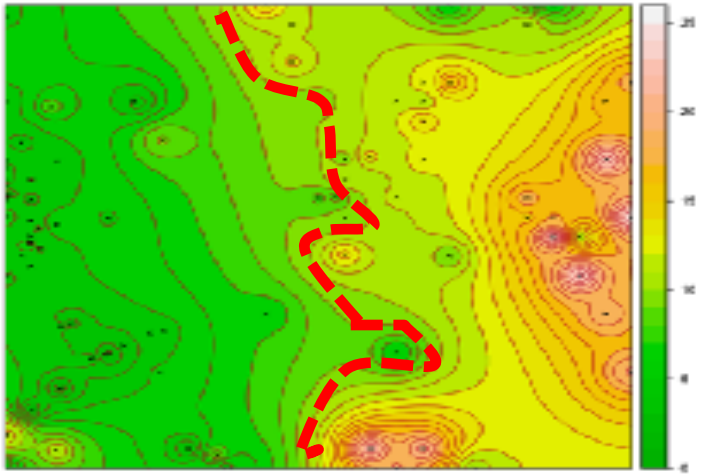
SPACE = objects + metric

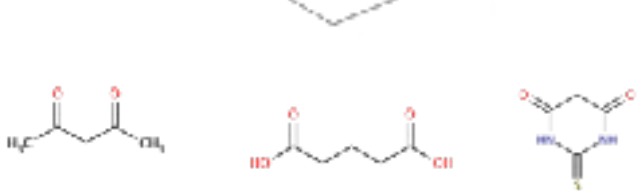
© A. Varnek

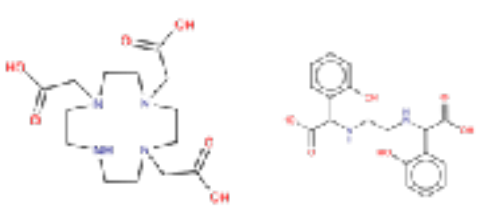
Chemical Space Representation and Vizualization

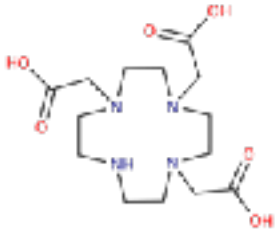
Desired property = *f* (structure + properties descriptors)









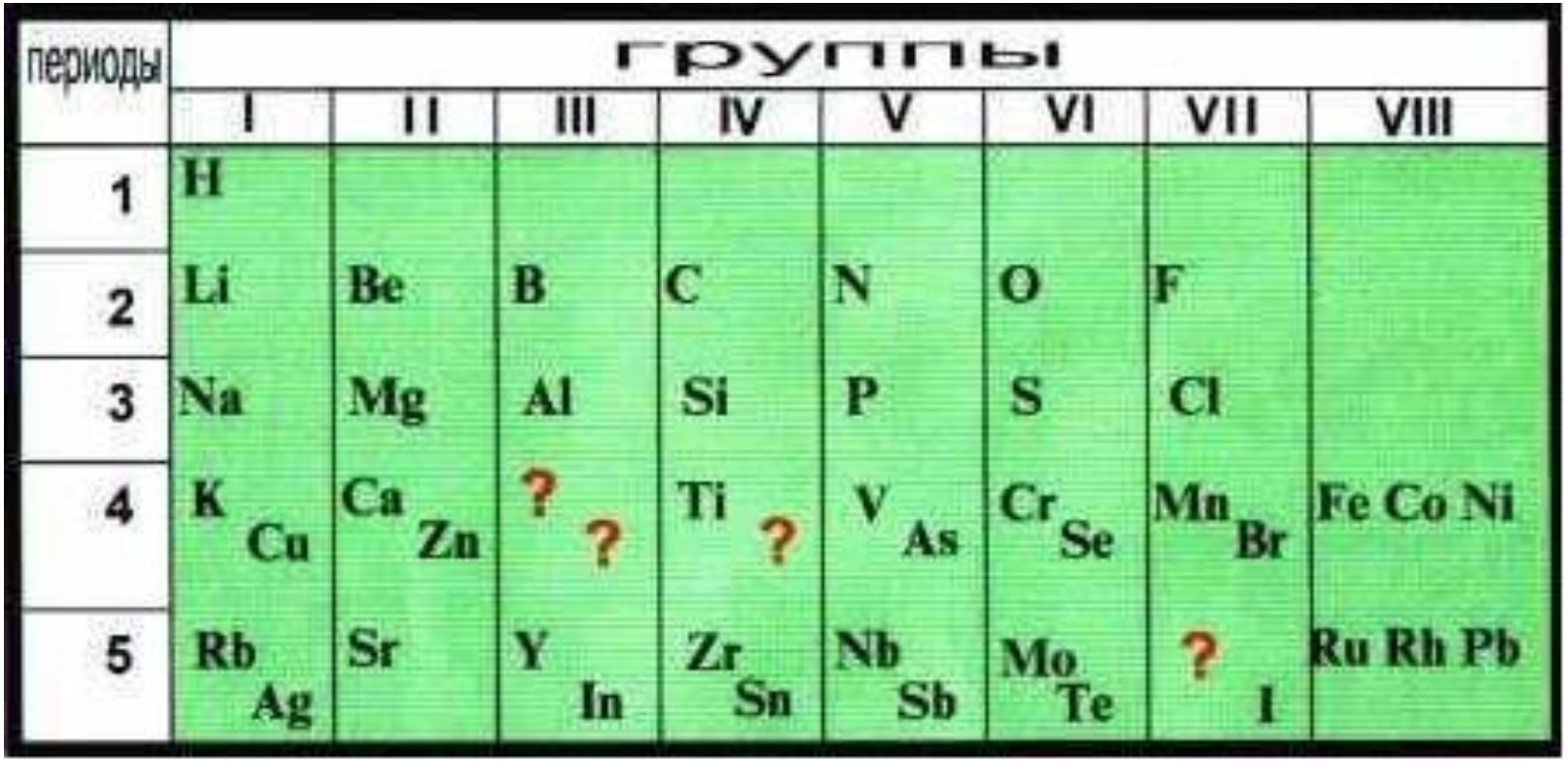


+ Lu^{3+}

Example: search for Lu^{3+} binders

H. A. Gaspar , I. I. Baskin, G. Marcou, D. Horvath, A. Varnek *Mol. Informatics,* 2015

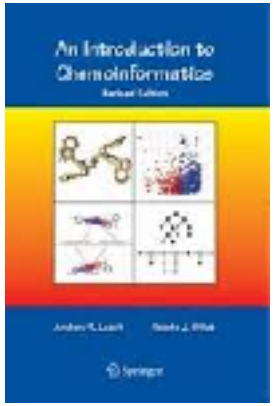
Pre-informatics: Periodic Table and Prediction of new elements

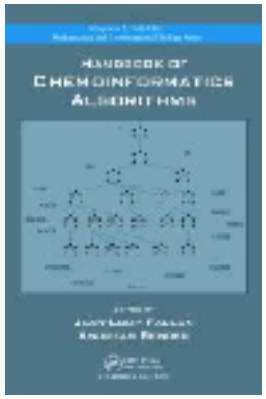


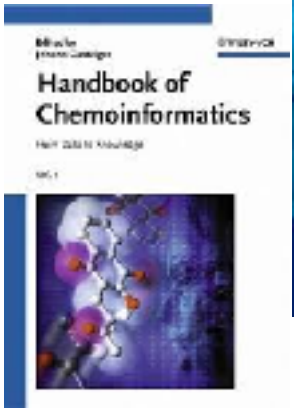
периоды	группы							
	I	II	III	IV	V	VI	VII	VIII
1	H							
2	Li	Be	B	C	N	O	F	
3	Na	Mg	Al	Si	P	S	Cl	
4	K Cu	Ca Zn	? ?	Ti ?	V As	Cr Se	Mn Br	Fe Co Ni
5	Rb Ag	Sr	Y In	Zr Sn	Nb Sb	Mo Te	? I	Ru Rh Pb

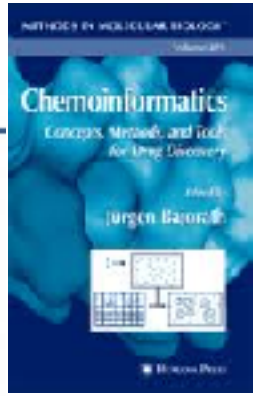
Mendeléev left space for new elements, and predicted four yet-to-be-discovered elements: Ga (1875), Sc (1879) Ge (1886) and Hf (1923) © A. Varnek

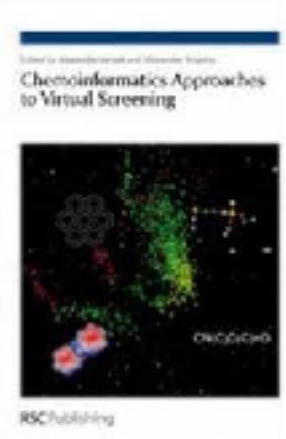
Selected Books in Cheminformatics

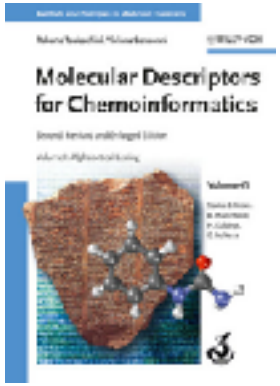


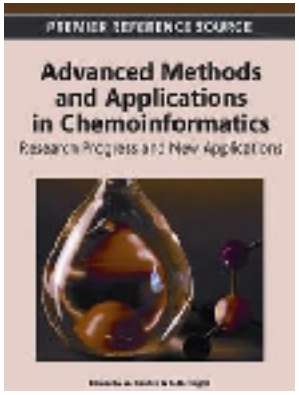


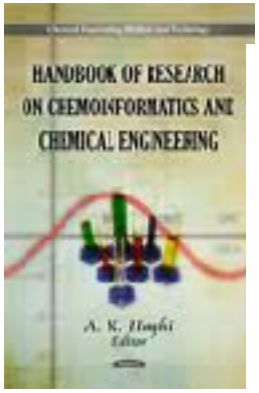


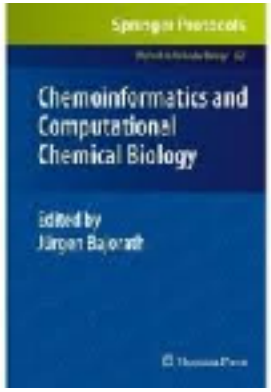










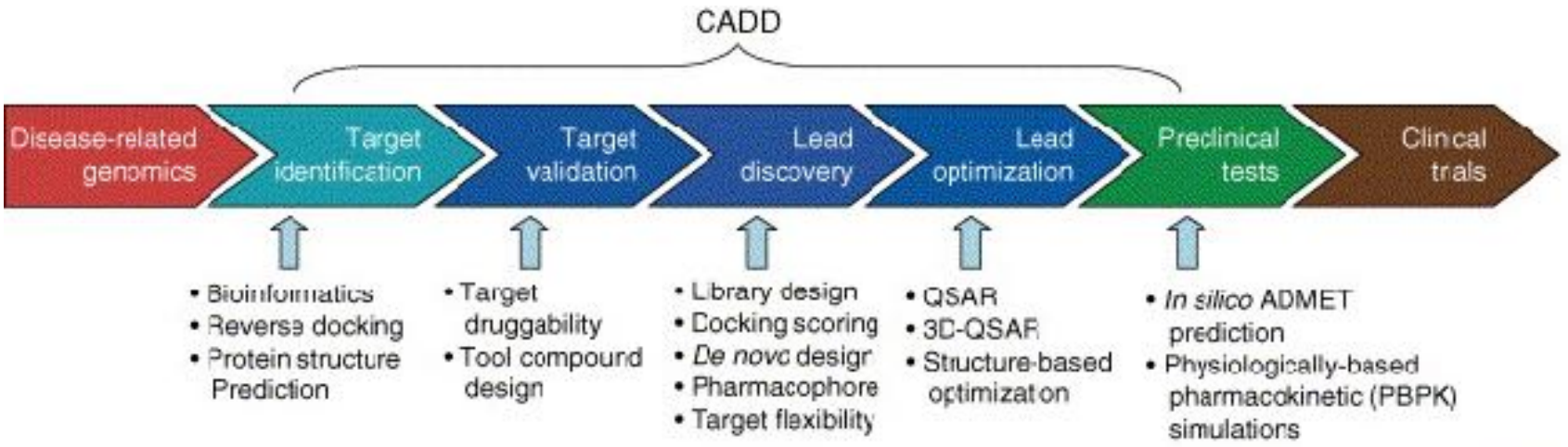


Anatoli Korkin
Nano & Giga Solutions

Computer-Aided Drug Design (CADD): Purpose

Accelerate the delivery of a drug candidate

- Identify hit compounds
- Support hit-to-lead progression
- Contribute to lead optimization
- Support other discovery activities



Drug Discovery Today: Technologies
Volume 3, Issue 3, Autumn 2006, Pages 307-313

Computer-Aided Drug Design (CADD): Toolkit

Virtual screening of commercially available or feasible compounds for potential hits

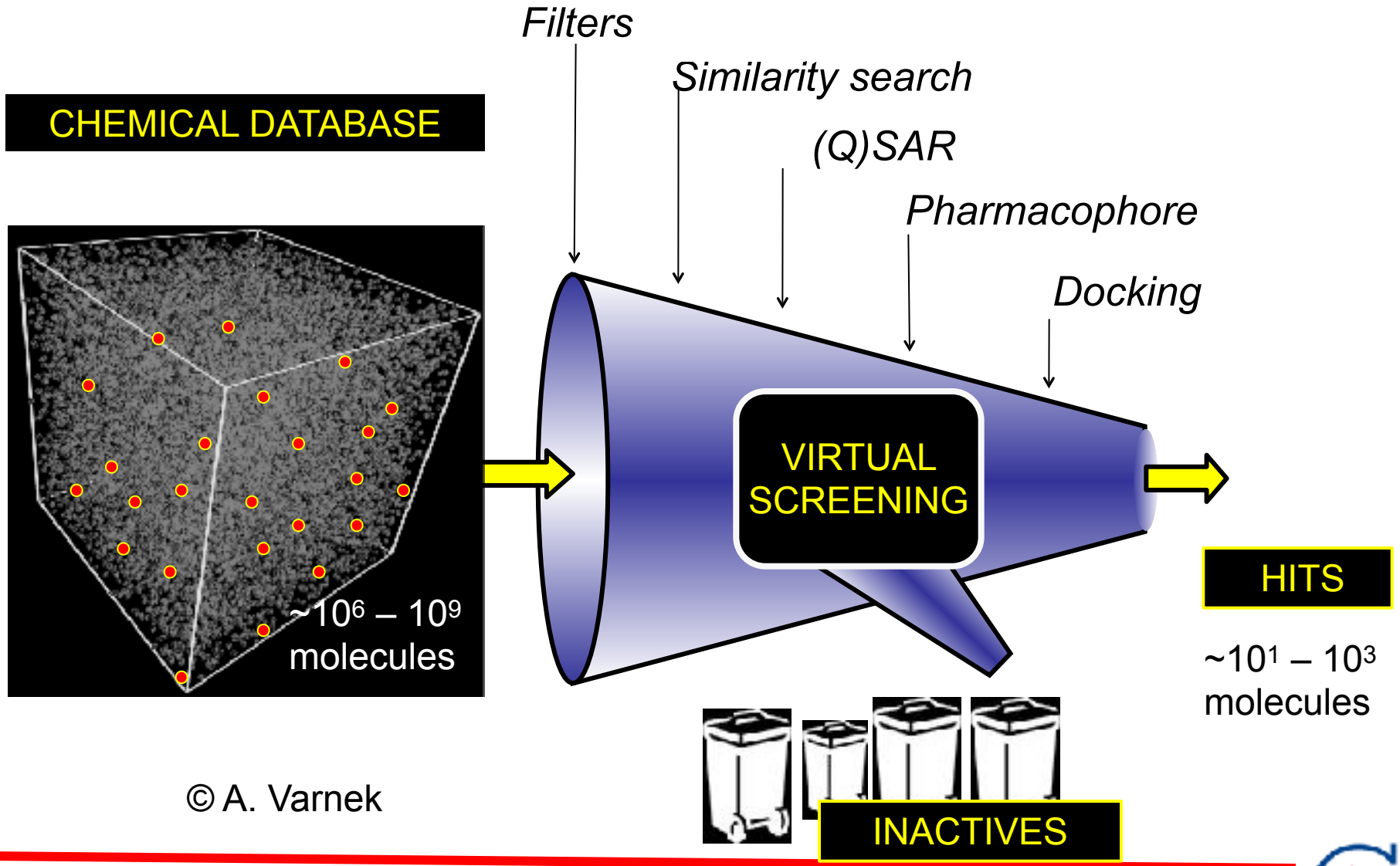
Structure-based design using 3D Models: Protein + potential drug

Molecular dynamics simulations of a protein's biological function and how it can be modulated by a drug molecule

In silico prediction of adsorption, distribution, metabolism and excretion

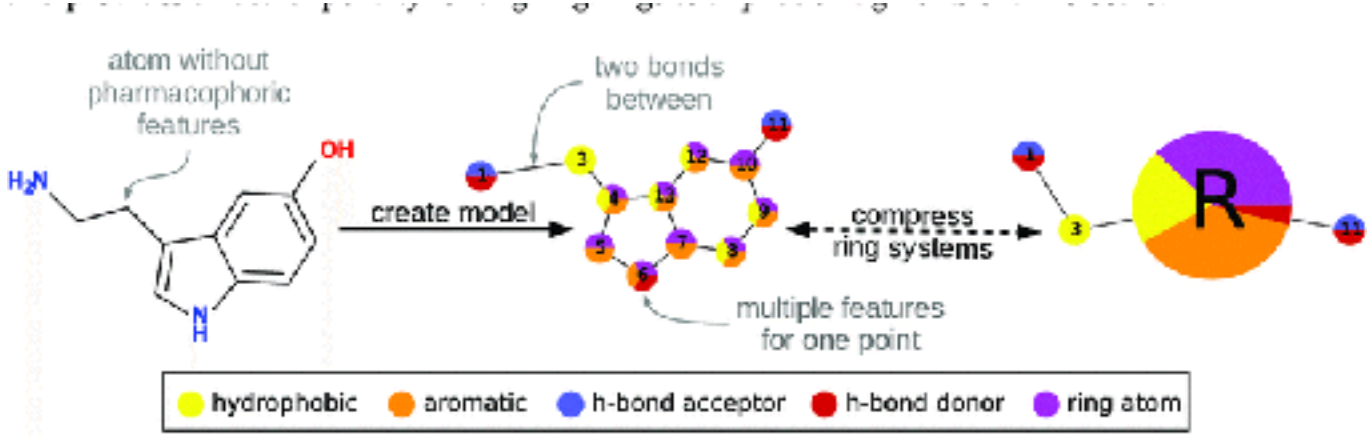
Chemoinformatics: Library design, data mining, Machine Learning

Virtual Screening “funnel”

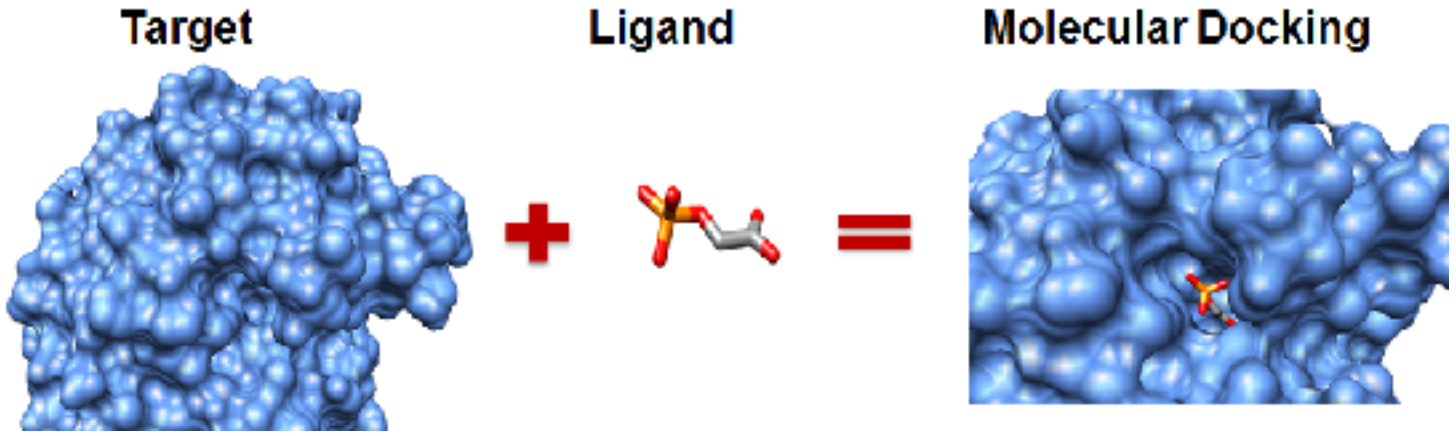


© A. Varnek

Pharmacophore and protein docking modeling

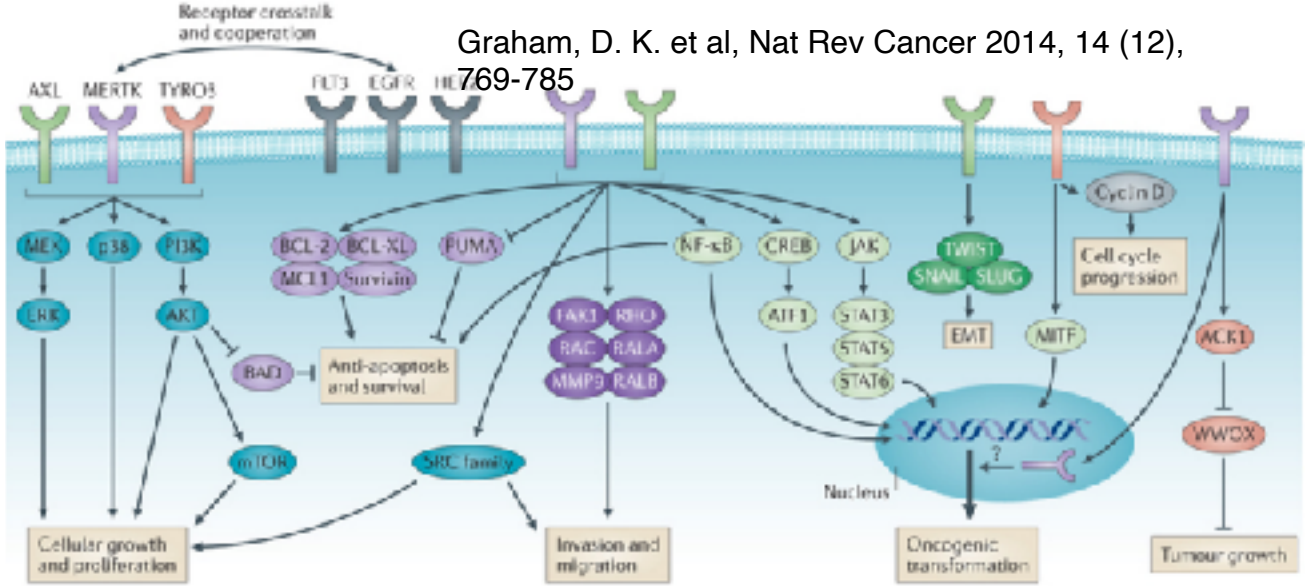


M. Stepniewska-Dziubinska, P. Zielenkiewicz, p. Siedlecki, Molecules 2017, 22(7), 1128



TAM-targeted cancer therapeutics

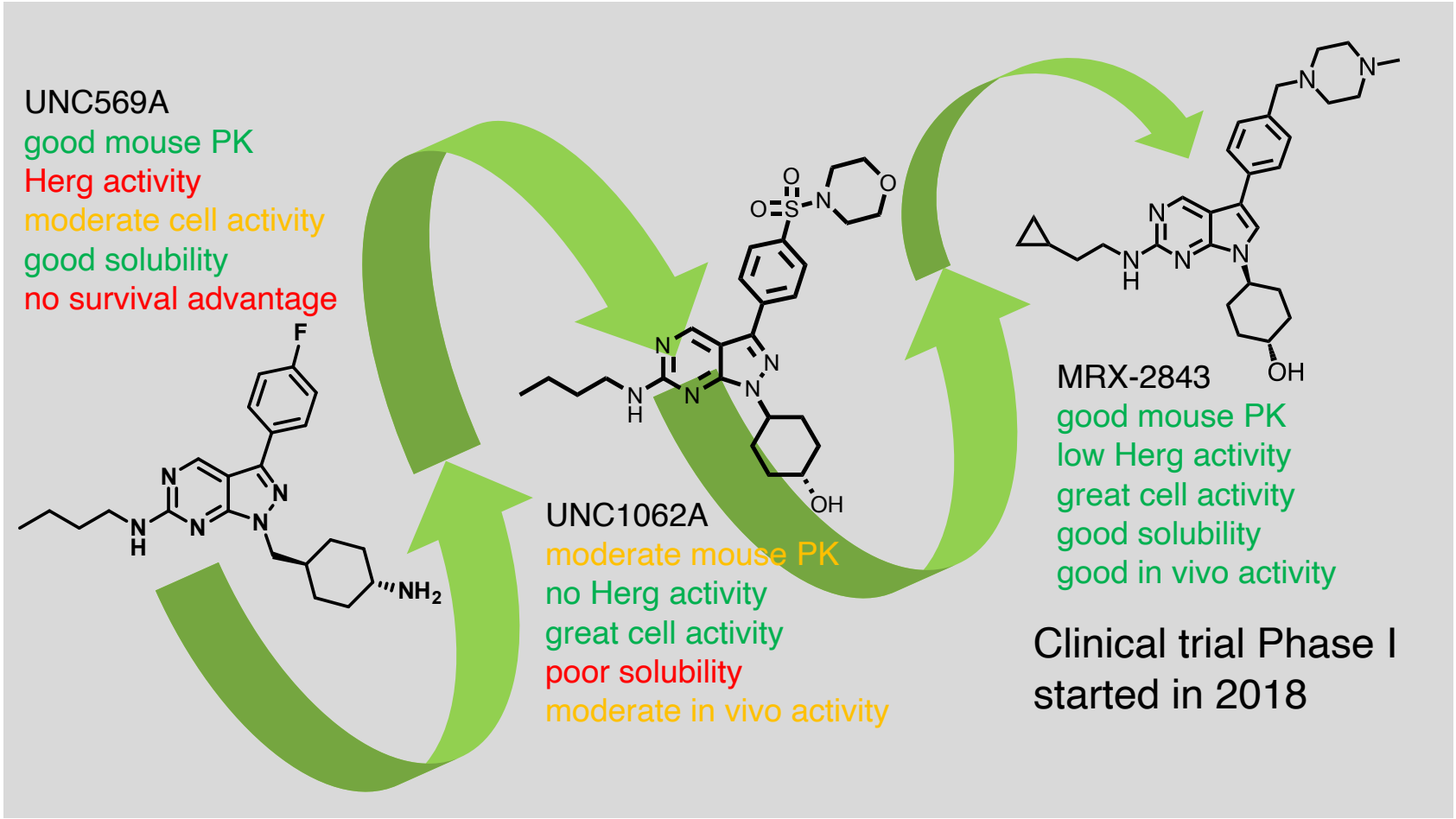
- Tyro3/Axl/Mer (TAM) RTK family
  - Expressed in monocytes to clear apoptotic material;
  - never expressed in normal T or B lymphocytes
- Expressed in human cancer
  - MER: 30-40% T cell Acute Lymphoblastic Leukemia (ALL);
  - MER/AXL: 41% B cell ALL and 68% pediatric AML
- Oncogenic function of ectopic expression
  - Survival signaling – anti-apoptosis
  - Critical for an “immune system” of a cancer cell
- Promising targets for cancer therapeutics



Graham, D. K. et al, Nat Rev Cancer 2014, 14 (12), 769-785

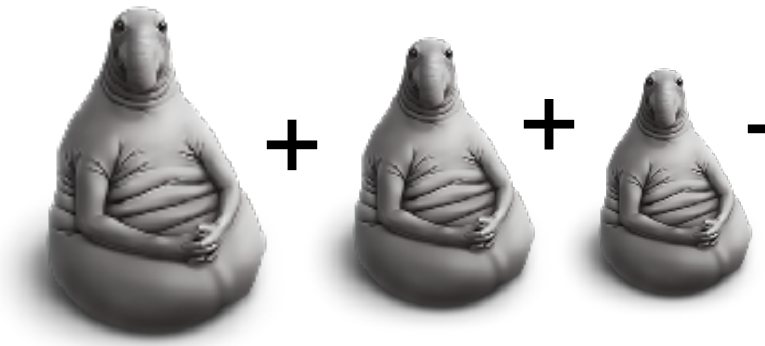
© D. Kireev

MER project evolution



© D. Kireev

Evolutionary algorithm

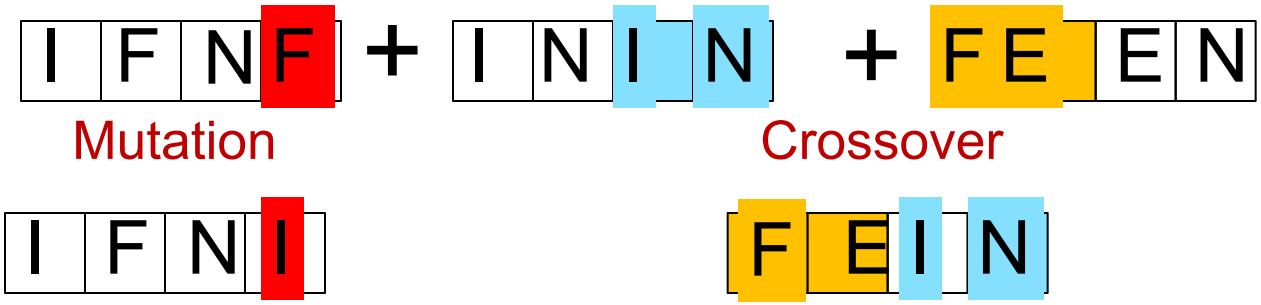


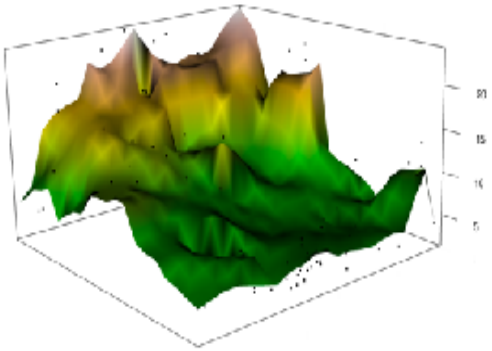
Initial population

Selection rules

Optimization

Champion

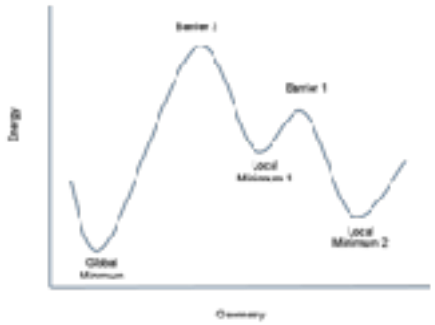




Material Design

Most stable Structure

Desired properties



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Genetic Algorithm applications in Materials Science

Design of self-assembling materials

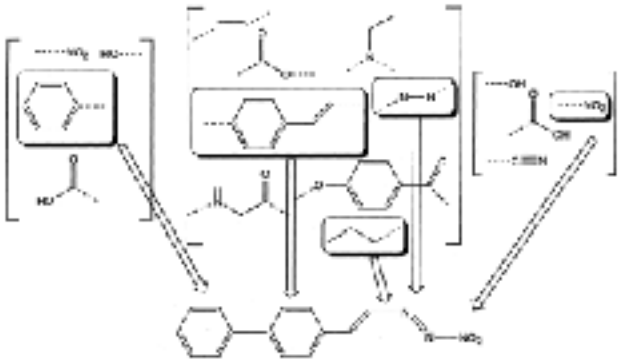


Fig. 4. Construction of a molecule from the building block library.

M. Keser and S.I. Stupp, Comput. Methods Appl. Mech. Engrg. 186 (2000) 373-385

Binary alloys design

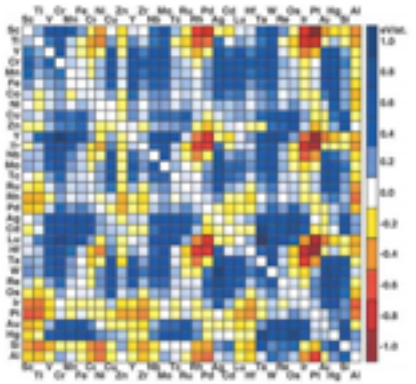
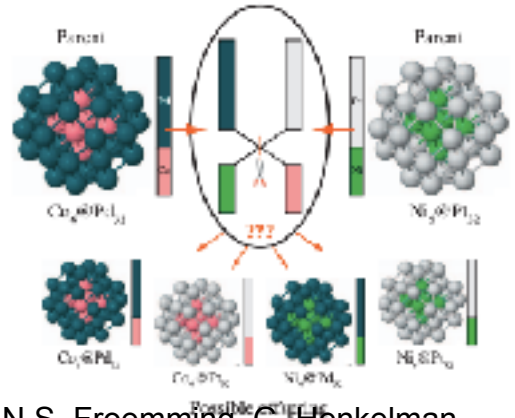


FIG. 2 (color). Enthalpies of formation for the fcc-like $L1_2$ structure of binary alloys. Horizontally are the elements of 75% abundance in the binary alloy, vertically are the elements of 25% abundance.

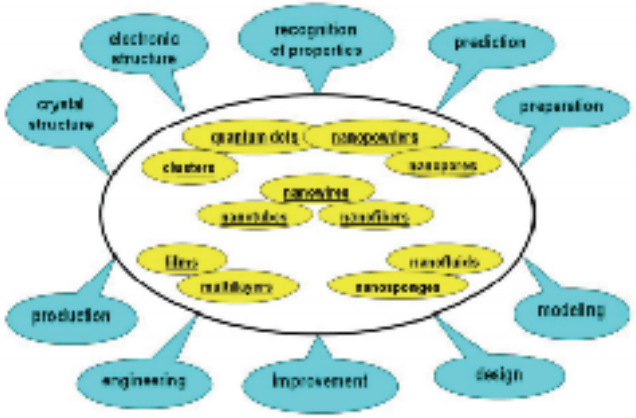
G.H. Johannesson et al, PhysRevLett. 88. 255506

Optimizing nanoparticle catalysts



N.S. Froemming, G. Henkelman, J. chem. Phys., 131, 234103, 2009

Review of applications in nanomaterials



W. Paszkowicz, Comp. methods in Mat. Sci. 2013, 13, 127-134

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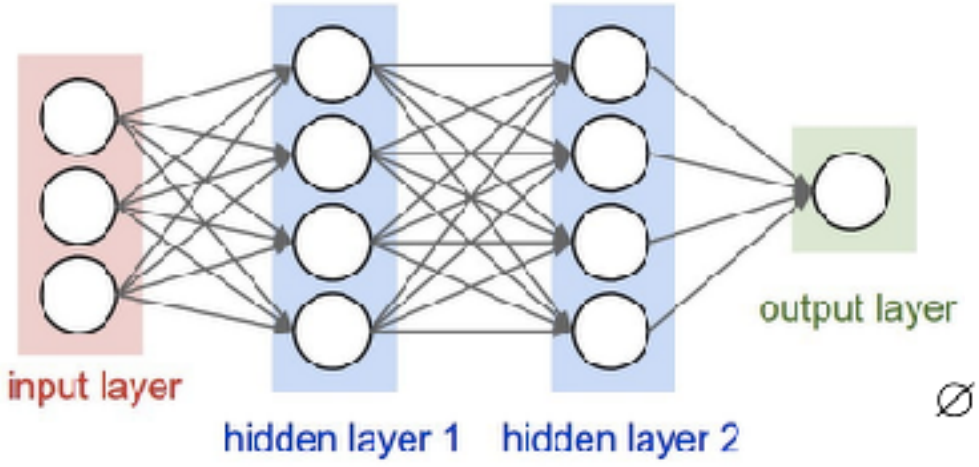
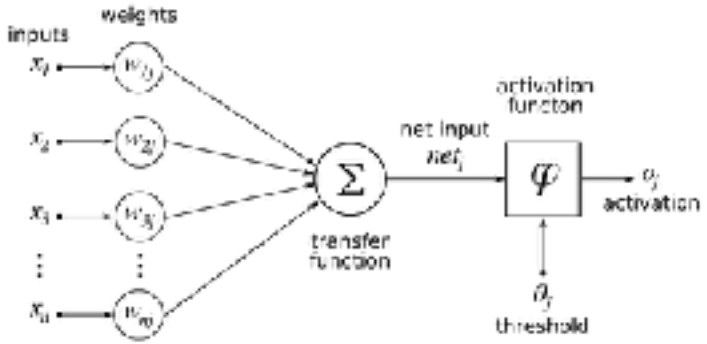
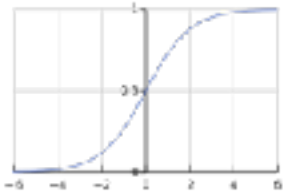
Artificial Neural Network



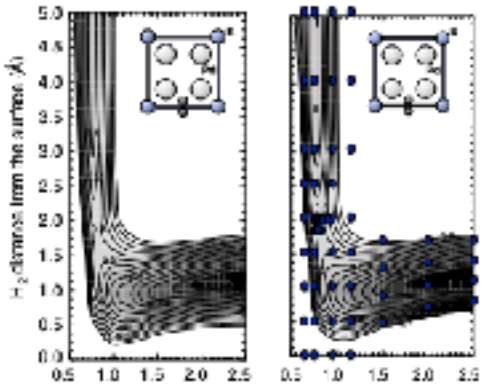


$$\varnothing(x) = \frac{1}{1+e^{-x}}$$



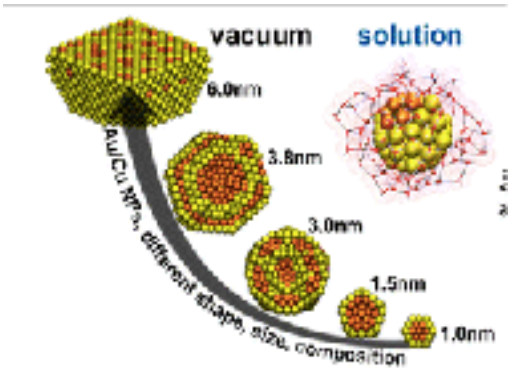
Training set => Back propagation algorithm => Finding weights

Surface reactions



S Lorenz, A Groß, M Scheffler , Chem. Phys. Lett., 2004, 395, 210-215

Nano-Au-Cu catalysts



N. Artrith, A. M. Kolpak, *Nano Lett.*, 2014, *14* (5), pp 2670–2676

Drug design

S. Agatonovic-Kustrin , R. Beresford, J.Pharm. Biomed. Analysis 22 (2000) 717–727

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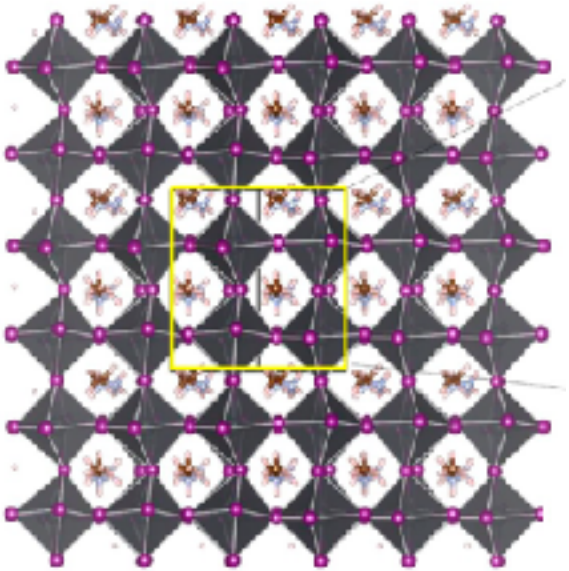
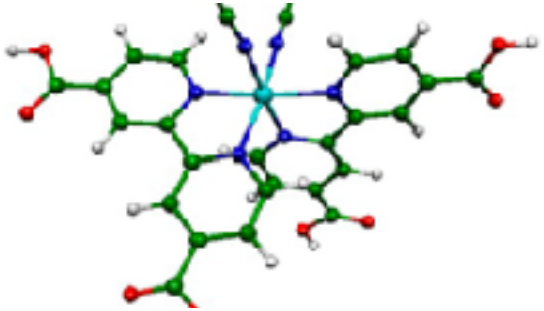
DFT Study of Dye-sensitized solar cells

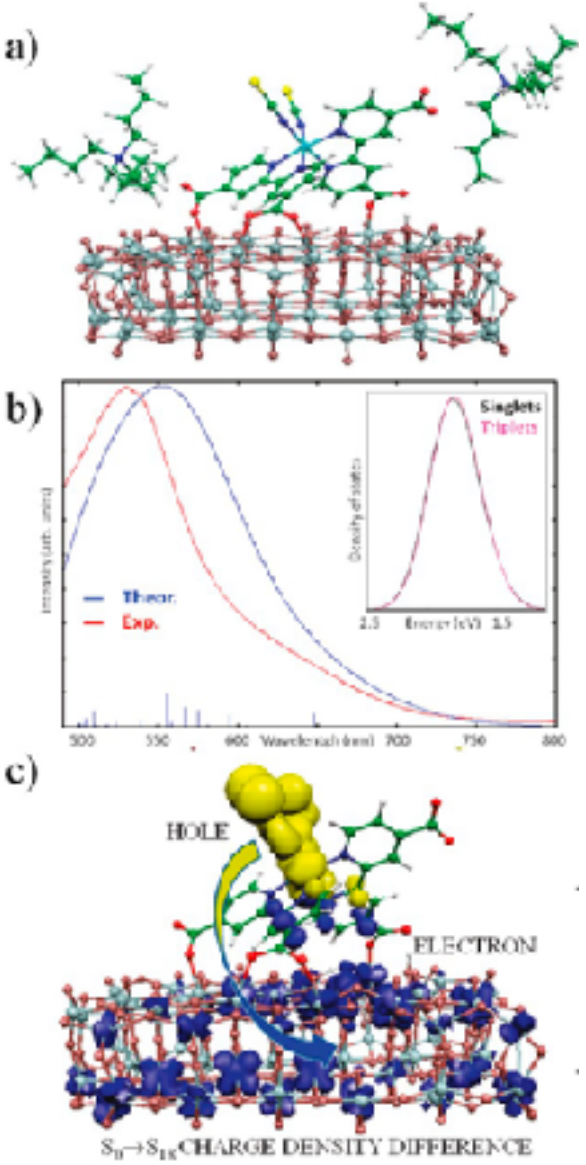


$MaPbI_3$ Structure



Ru(II)-polypyridyl complex

F. De Angelis, Acc. Chem. Res., 2014, 47, 3349



Ru(II)-complex on TiO_2

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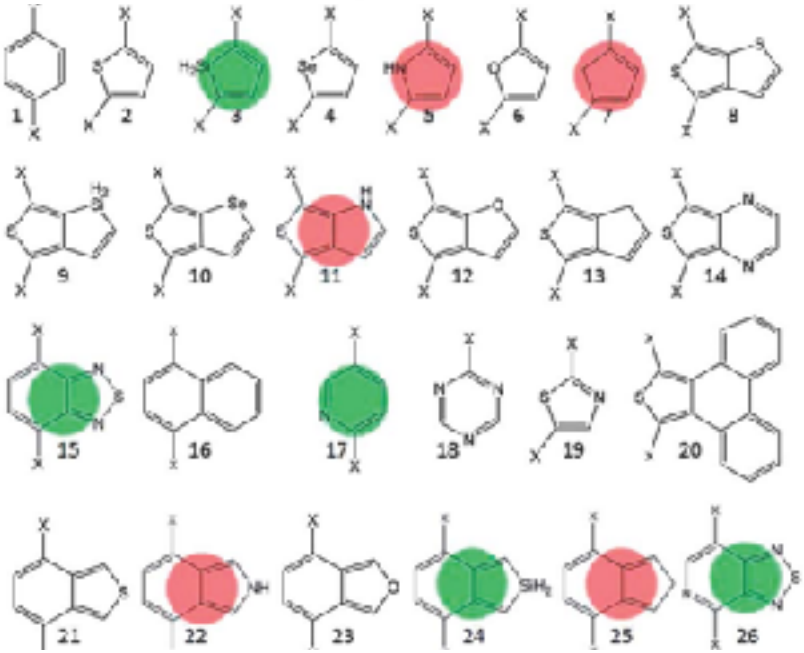
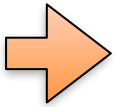
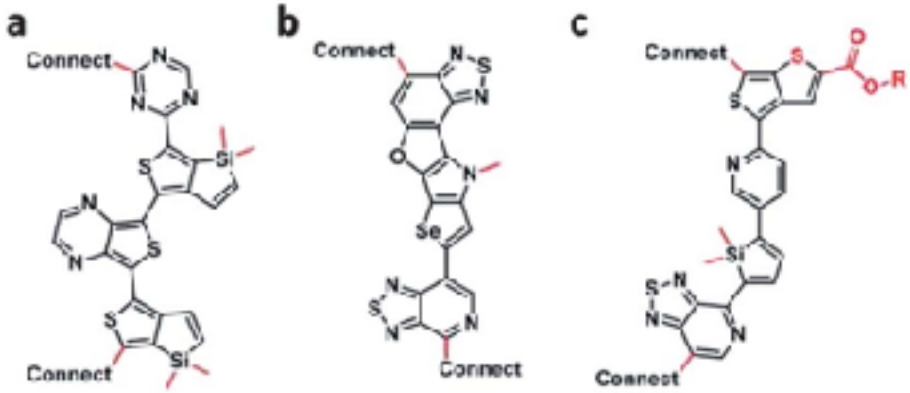
Computational screening of organic photovoltaics





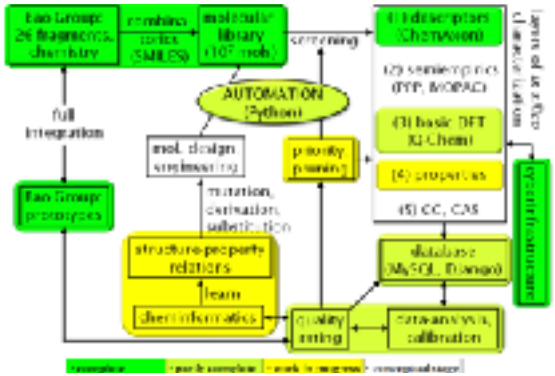


Leading candidates

DFT + Cheminformatics

2,3 millions of compounds from 26 blocks

IBM World Community Grid



Harvard Clean Energy Project

Hachmann et al, Energy Environ. Sci., 2014, 7, 698

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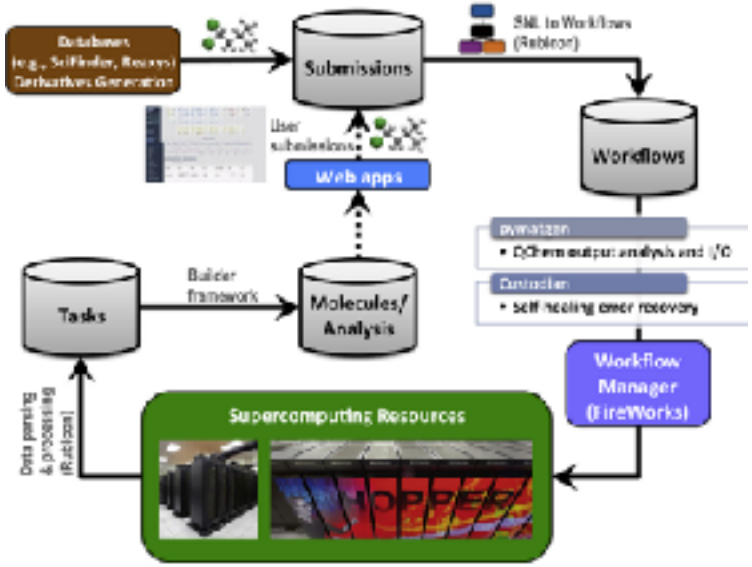
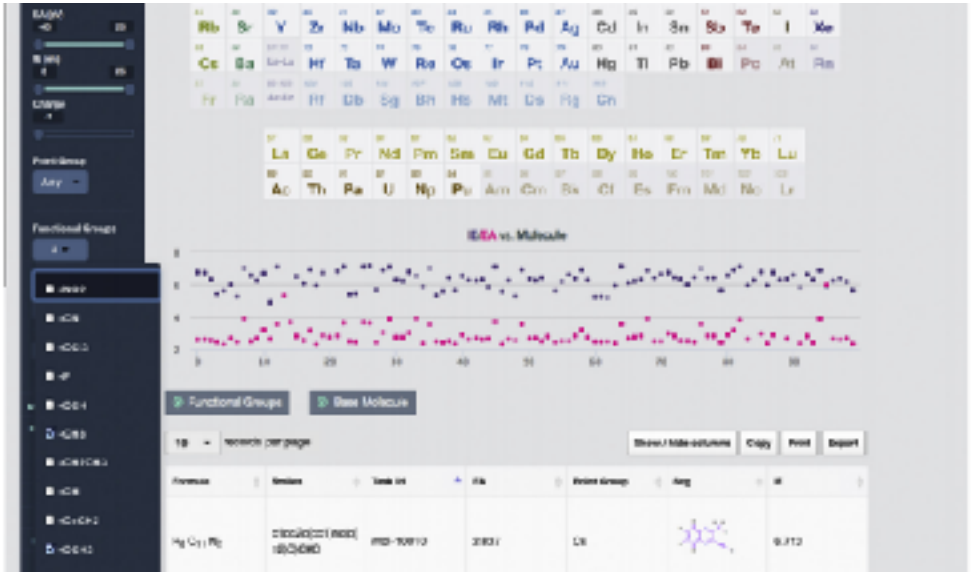
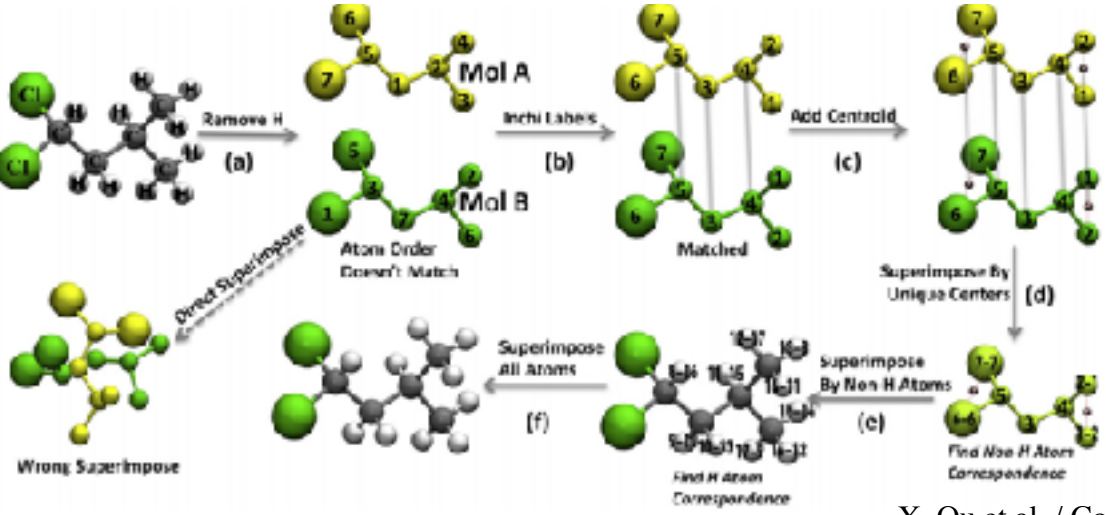
DFT + AI Screening of electrolytes for Li-batteries







Infrastructure and computations:

- 4830 IP/EAs and redox potentials

- pair dissociation constants

- salt complex structure

X. Qu et al. / Computational Materials Science 103 (2015) 56–67

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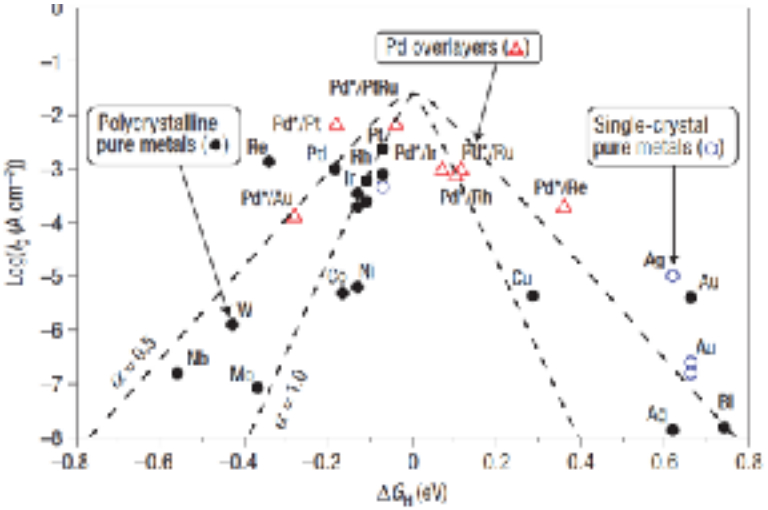
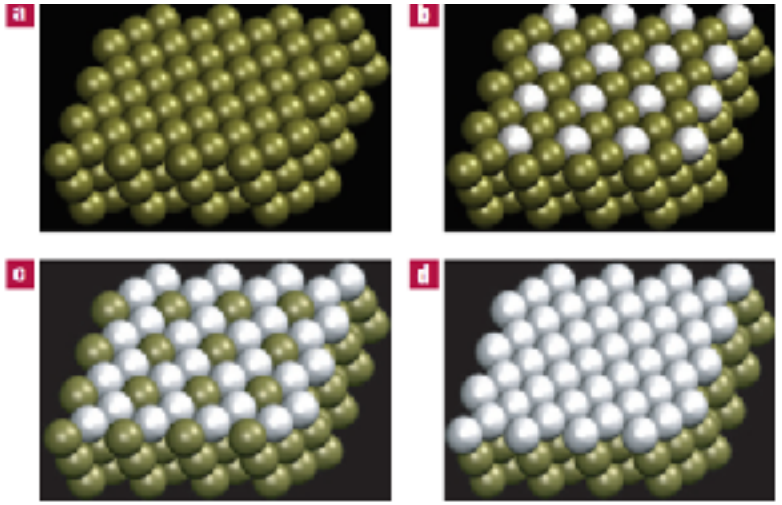
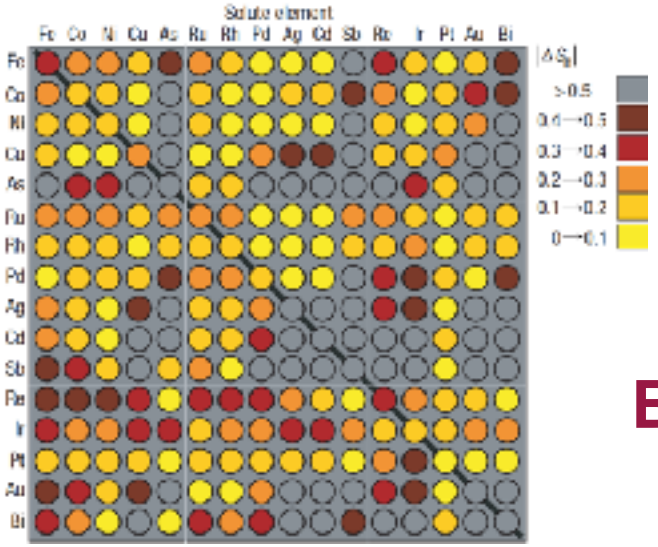
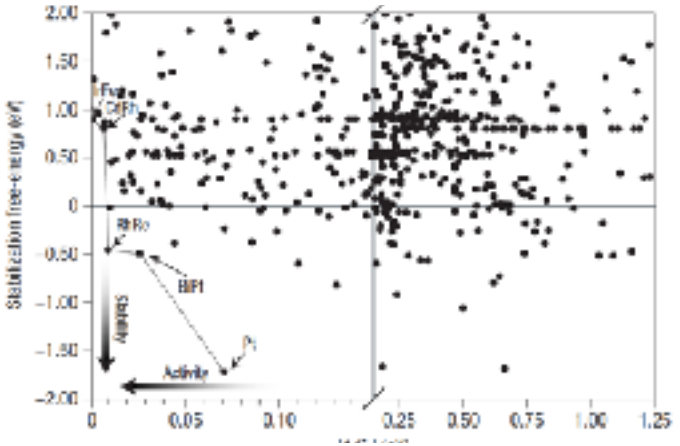
Computational high-throughput screening of electrocatalytic materials for hydrogen evolution







BiPt



Greeley et al, Nature Materials, 2006, 5, 909

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Thank you for your attention

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