materials design®

The MedeA® Software Platform: Overview and Applications

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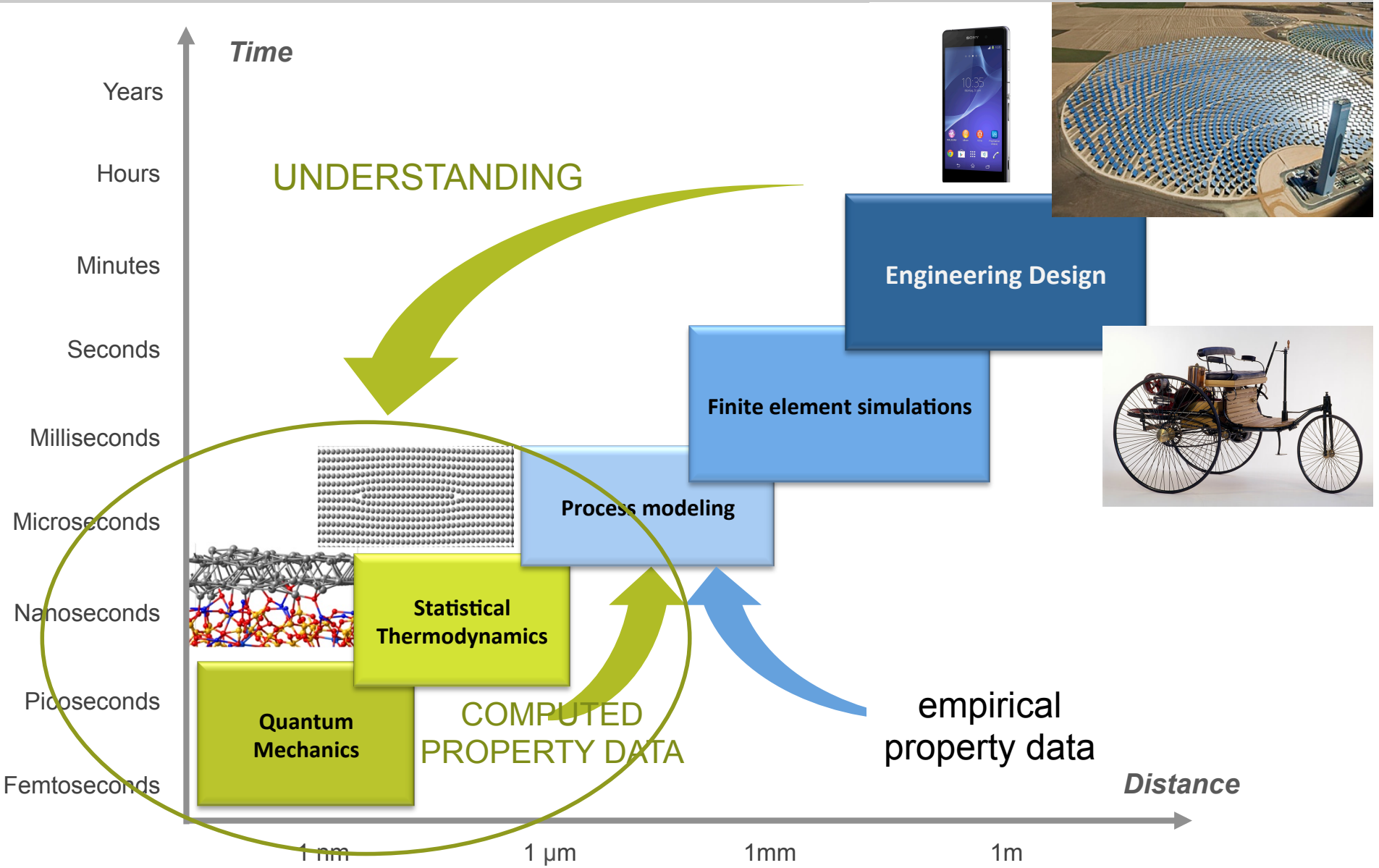
Materials Design Inc.

Thermoelectric Network Meeting
Reading
11-12 November 2015

Agenda

- Company Profile Materials Design
  - Products and Services: Software and Consulting
- Challenges and Solutions
  - Capabilities of the MedeA® software environment
- Selected Applications
  - Electronic properties
  - Phonon dispersions
  - Transport properties
- Discussion and Software Demonstration

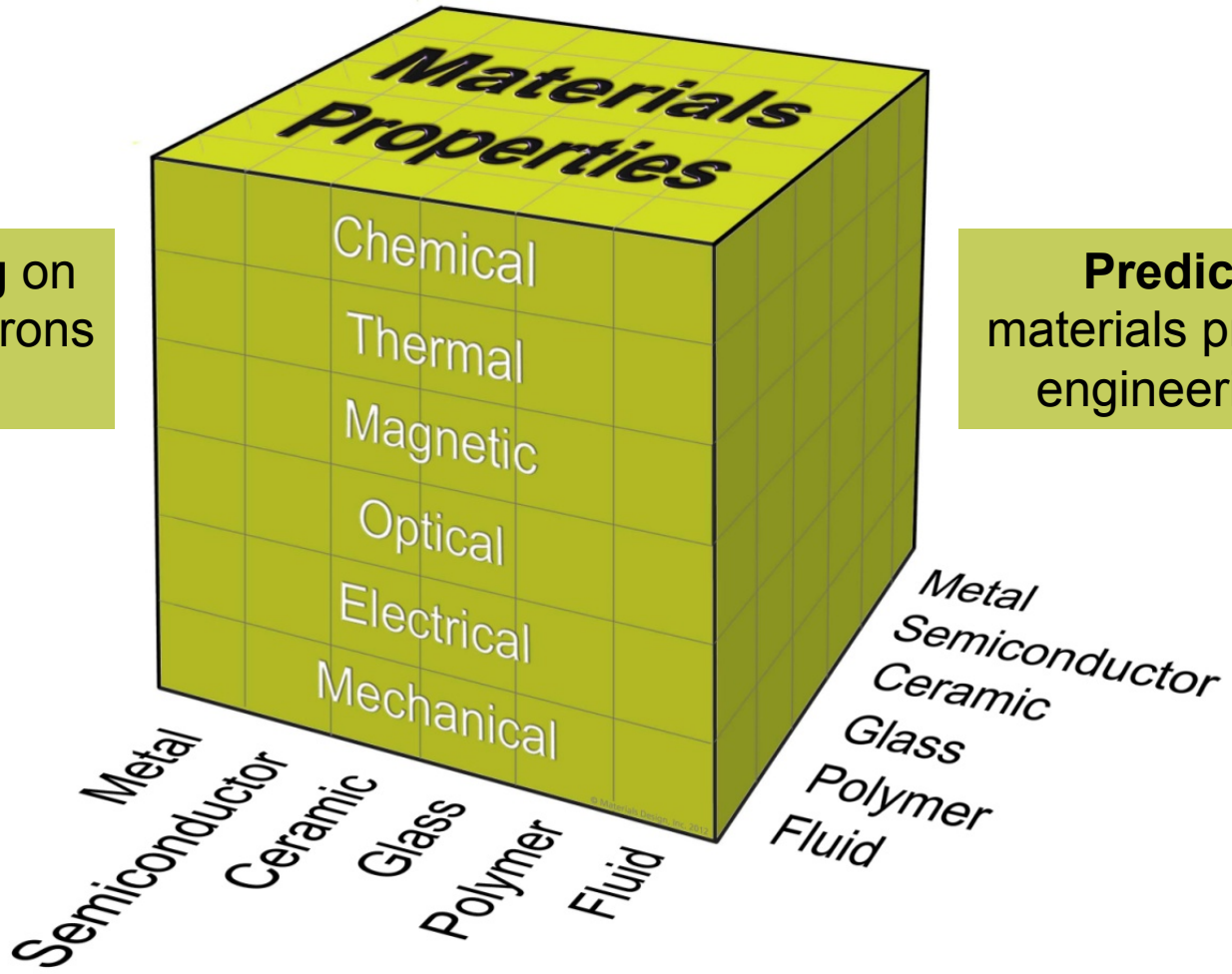
Technology Positioning



Goal of Atomistic Simulations

MedeA®: Software for Efficient R&D

Understanding on the level of electrons and atoms



Prediction of materials properties of engineering value

Company Profile

- Founded by scientists in 1998
- Over 400 customers in industry, universities, and government laboratories including over 50 major companies worldwide
- Products: **MedeA**® software, support, and consulting services
- Global: Offices in San Diego, Angel Fire, Paris, and Stockholm
- Business partners: Japan, Korea, China, Taiwan, Singapore, and India
- Core competence in
  - Computational chemistry & physics
  - Materials science & chemical engineering
  - Materials property databases & software engineering

Products and Services

- **MedeA® software**
  - Comprehensive atomistic modeling environment with leading technology
  - Installation, training, online support, and maintenance
  - Scientific/technological interactions
  - Users group meetings

- **Contract research**
  - Solution of specific industrial problems
  - Leverages expertise and resources of MD's scientists
  - Publicly funded programs
- **Technology partnerships**
  - Development of customized modeling capabilities (e.g. Toyota)

Customers

Energy	Metals & Alloys	Chemicals	Oil & Gas
Electronics	Automotive & Aerospace	Glass & Ceramics	Mining & Drilling
Universities and Government R&D Laboratories			

Materials Exploration and Design Analysis

MedeA® Software

MODELING & ANALYSIS

Builders: crystals, defects, interfaces, surfaces, molecules, nanostructures, polymers, amorphous materials

Analysis: geometry, band structures and DOS, electron and spin density, potential, Fermi surface, phonons, transition states, dynamics trajectories

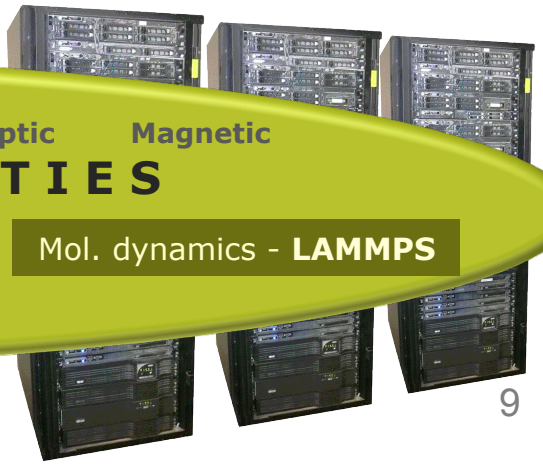
Job Server

DATABASES

Experimental and Computed Structure and Property Data

ICSD | NIST Crystal Data | Pauling | Pearson | Computed

Task Servers



Mechanical Thermal Chemical Kinetic Electric Optic Magnetic

COMPUTATION OF PROPERTIES

ab initio QM - **VASP** | Semi-empirical - **MOPAC** | Monte Carlo - **GIBBS** | Mol. dynamics - **LAMMPS**

MedeA® Components

- **MedeA®-Environment**
  - Model builders
  - Database infrastructure
  - Analysis tools
  - Flowcharts
  - JobServer/TaskServer
- **InfoMaticA**
  - About 500,000 database entries combining ICSD, Pearson, Pauling, NIST Crystal Data, COD
  - Computed data
- **VASP**
  - GGA , post-DFT (hybrid, sX, GW, RPA)
  - H to Cm PAW potentials (all electron)
  - Spin-orbit relativistic
  - Linear response
- **LAMMPS**
  - Forcefields including pcff+, ionic, EAM
- **GIBBS**
  - Adsorption
  - Fluid phase equilibria
- **MOPAC**
  - Semi-empirical QM, PM7
  - Thermodynamics, IR, UV-vis

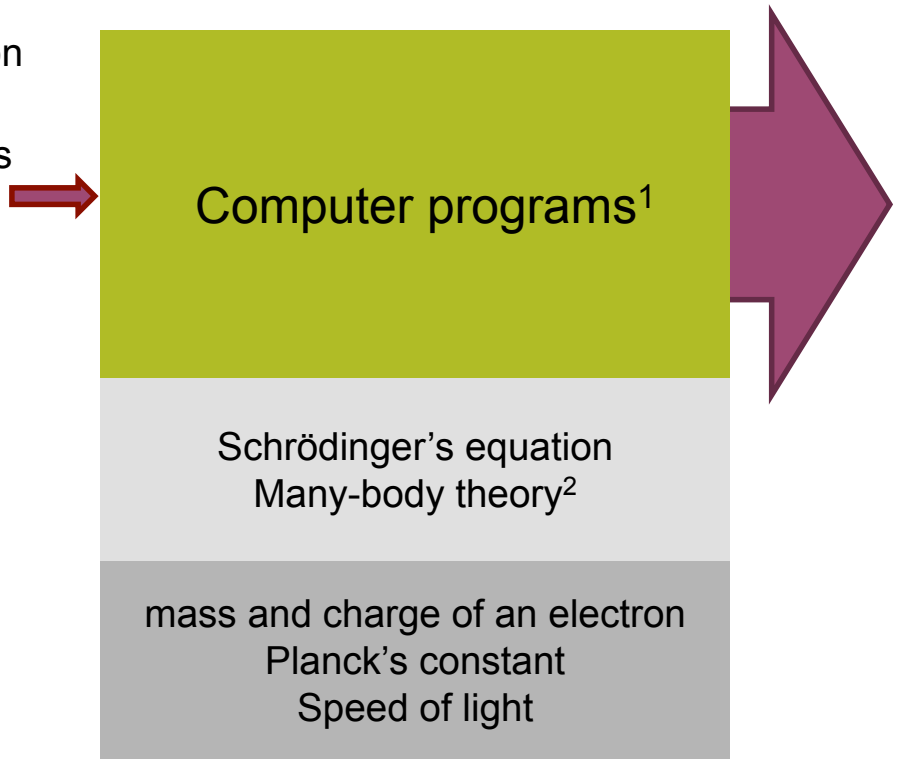
Property Packages

- Mechanical-Thermal (MT)
- Phonon
  - Phonon dispersions
  - Vibrational properties
  - Thermodynamic functions
- Electronics
  - Effective masses
  - Boltzmann transport
  - Electrical/thermal conductivity
  - Thermoelectricity
- Transport
  - Diffusion
  - Thermal conductivity
  - Viscosity
- Transition State (TSS)
- Amorphous materials
- Polymer properties
  - QSPR
- PrediBond™ – catalysis

Ab Initio Methods

INPUT

- Arbitrary position of atomic nuclei
- Atomic numbers
- Atomic masses



$$\mathbf{H}\Psi = E\Psi$$

OUTPUT

- Interatomic distances
- Lattice parameters
- Stress
- Thermodynamic stability
- Defect energies
- Surface energies
- Grain boundary energies
- Adsorption energies
- Binding energies of impurities
- Reaction barriers
- Diffusion rates
- Electronic, optic, and magnetic properties
- …

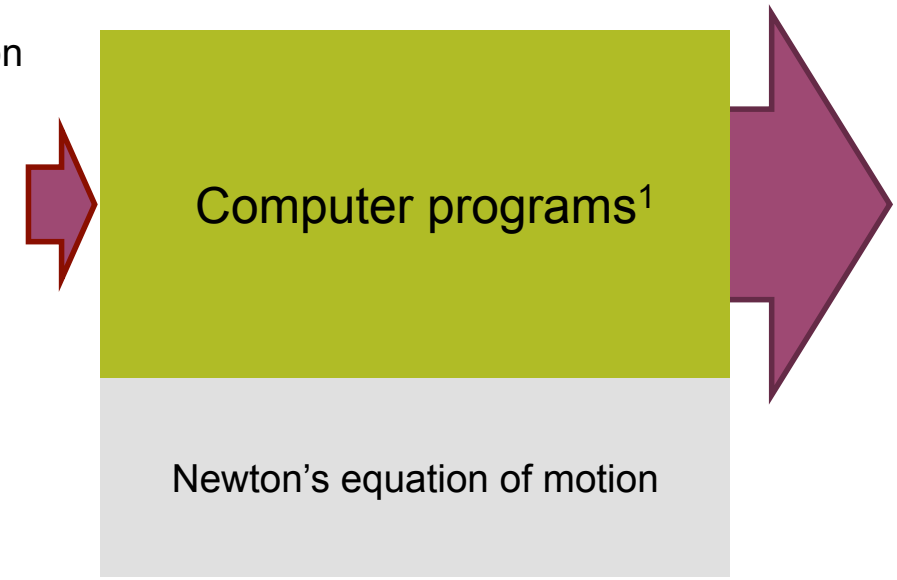
1. Vienna Ab initio Simulation Package (VASP)
2. Density functional theory (DFT)

- free of system-specific parameters
- general and high predictive power
- few hundred atoms per simulation box
- very short time scales (pico-seconds)

Forcefield Methods

INPUT

- Arbitrary position of atomic nuclei
- Atom types
- Atomic masses
- Parameters for interatomic interactions



OUTPUT

- Interatomic distances
- Lattice parameters
- Stress
- Thermodynamic stability
- Defect energies
- Dislocations
- Surface energies
- Grain boundary energies
- Diffusion rates
- …

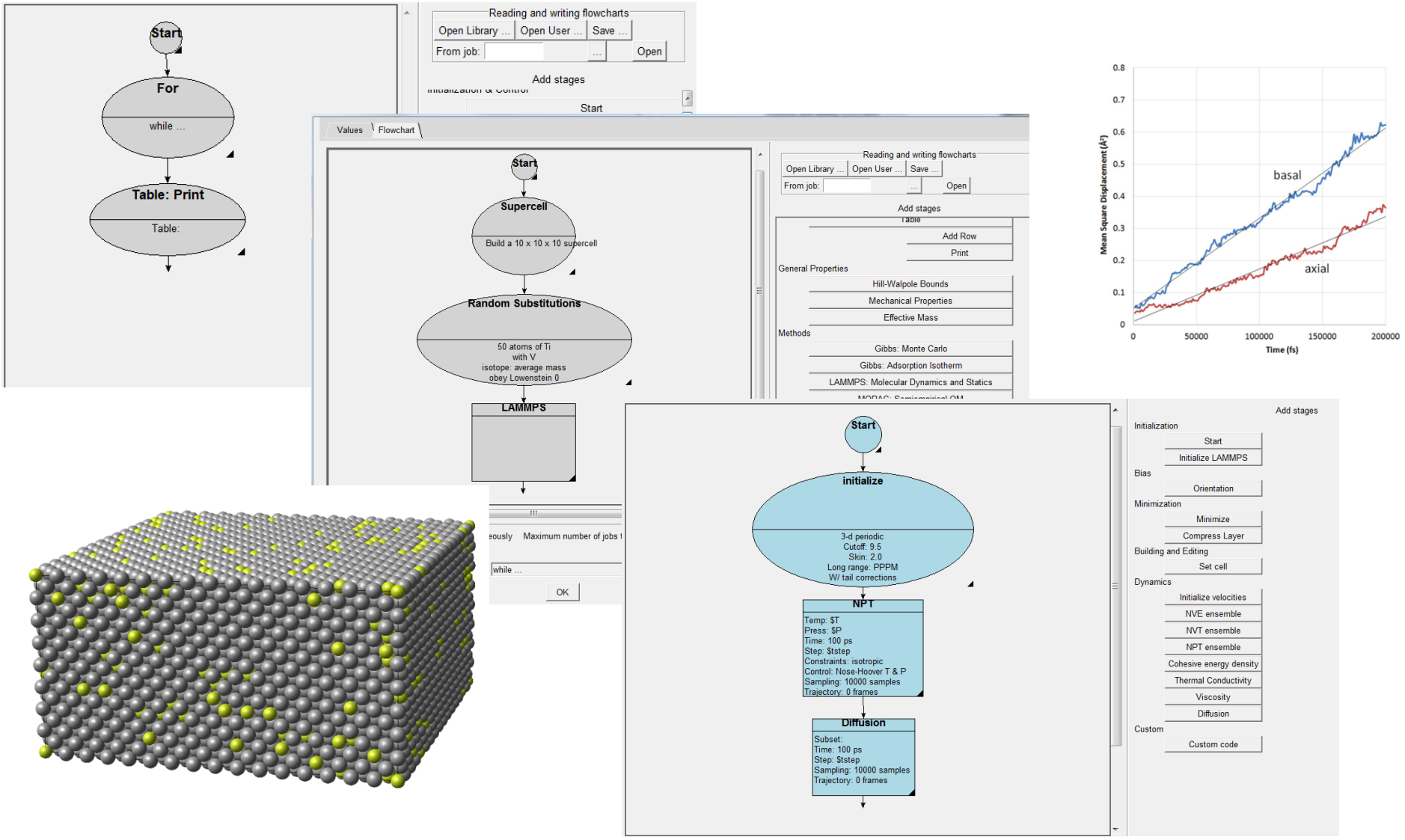
$$F = m\frac{\partial^2 E}{\partial x^2}$$

$$E = \sum_{i,j} V_{bonds}\left(r_{ij}\right) + \sum_{i,j,k} V_{angles}\left(\theta_{ijk}\right) + \ldots$$

- system-specific parameters fitted to ab initio or experimental data (MedeA®-FFO)
- predictive within range of fitting parameters
- up to millions of atoms per simulation box
- time scales into the nano-seconds
- no electronic structure-related properties

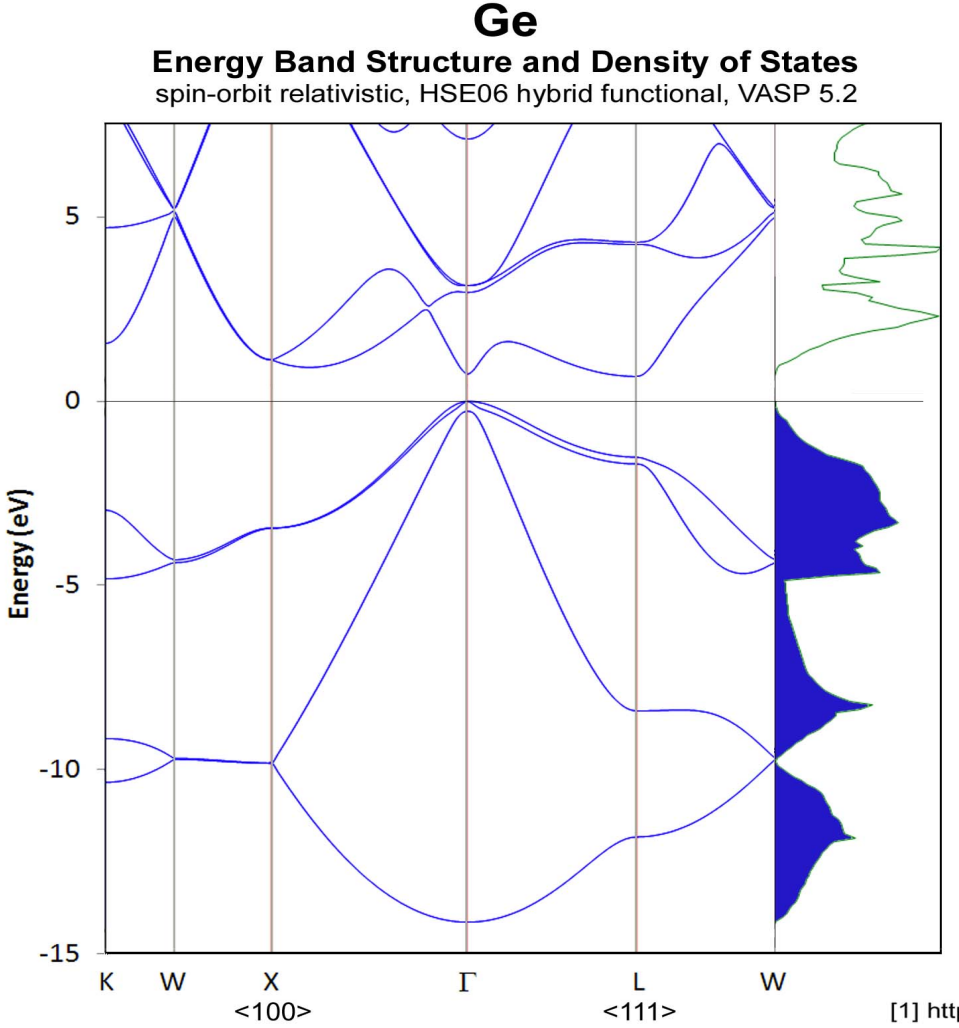
1. Large-scale Atomic/Molecular Massively Parallel Simulator (LAMMPS)

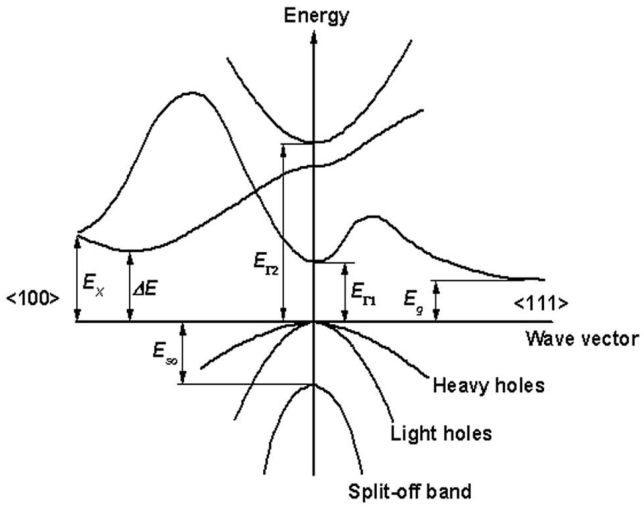
Flowcharts



Electronic Properties, Band Gaps

Accurate Band Structures



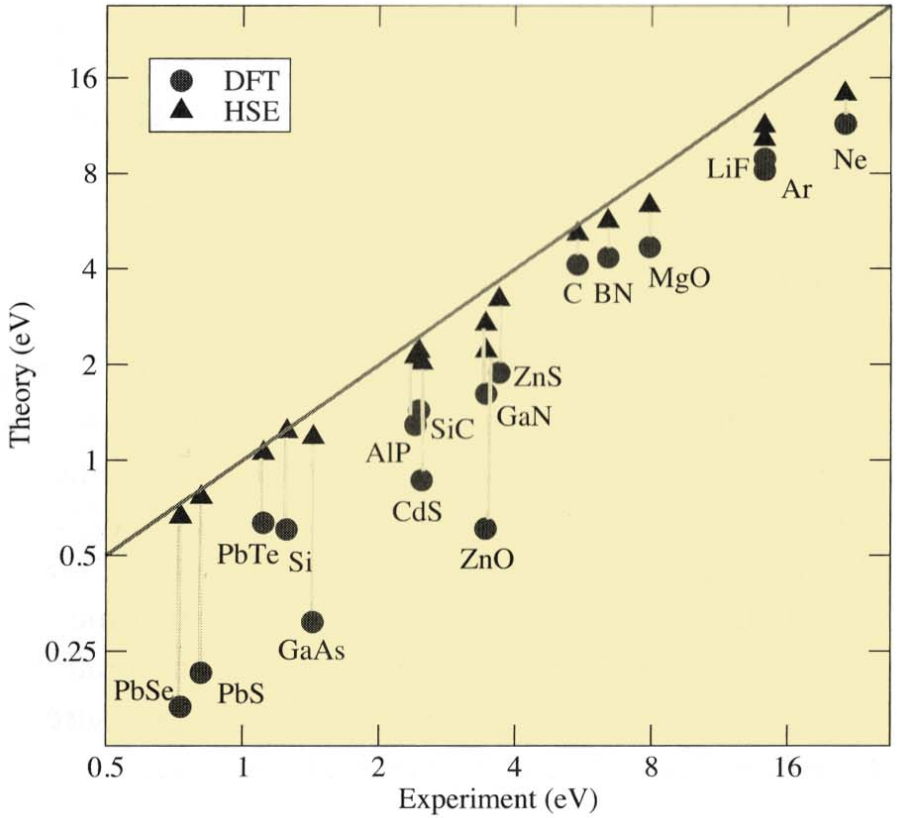


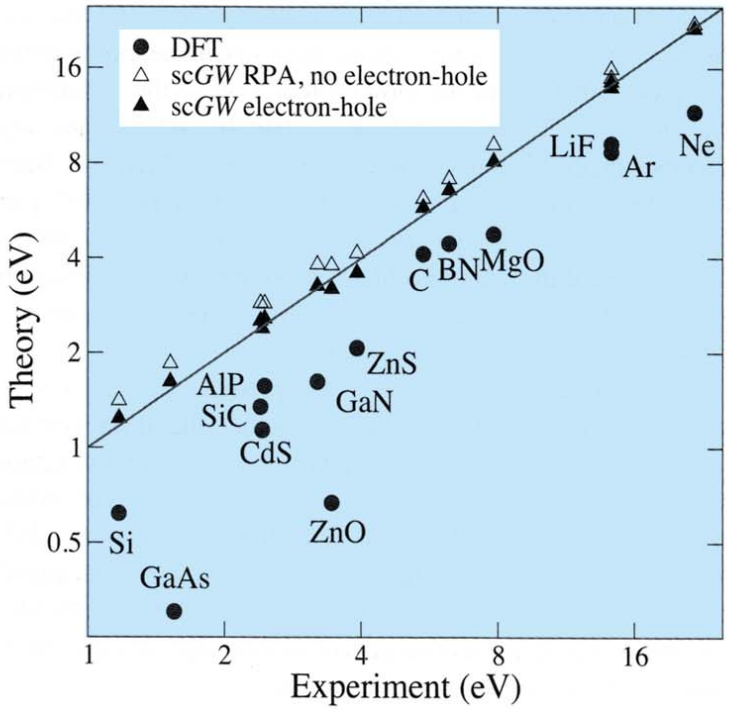
		Expt. [1]	Computed
300 K	E_g	0.66 eV	0.66
	E_X	1.2 eV	1.12
	$E_{\Gamma 1}$	0.8 eV	0.73
	$E_{\Gamma 2}$	3.22 eV	3.14
	ΔE	0.85 eV	0.91
	E_{so}	0.29 eV	0.29

[1] http://www.ioffe.rssi.ru/SVA/NSM/Semicond/Ge/bandstr.html

Note: Standard LDA or GGA predicts Ge to be metallic

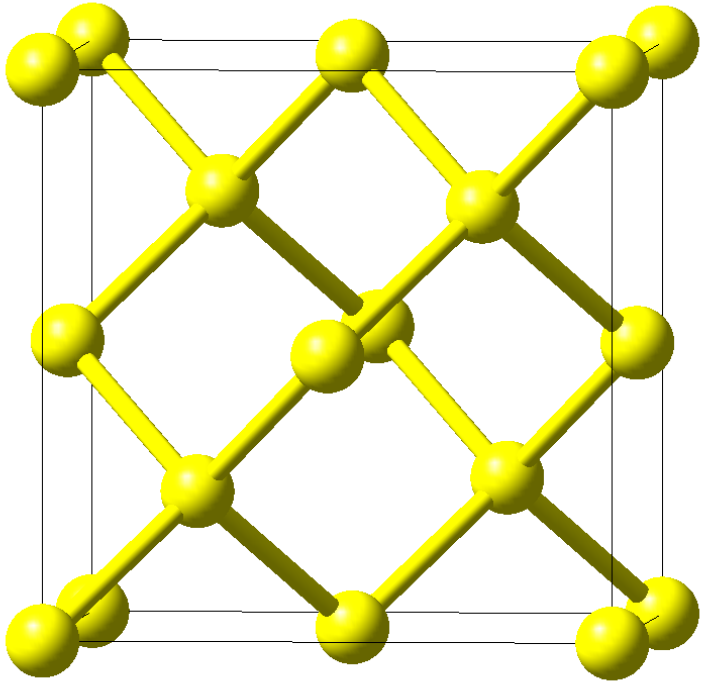
Accuracy of Computed Band Gaps



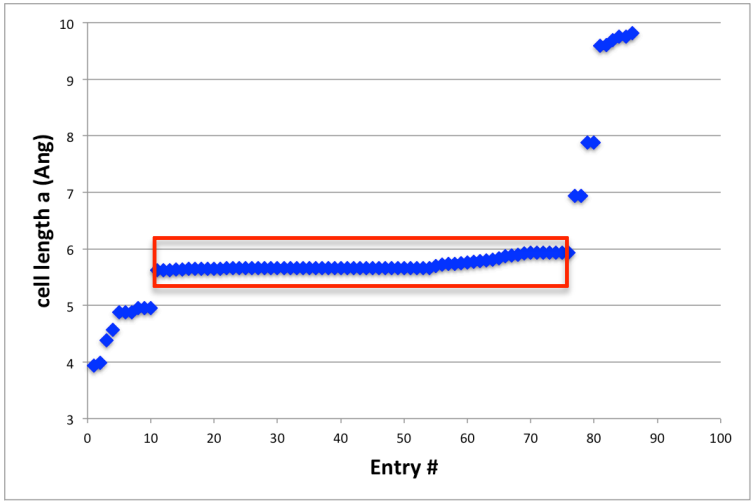


Performance of VASP 5.2 as reviewed by
J. Hafner, J. Phys.: Cond. Matter **22**, 384205 (2010)

Germanium: Atomic Structure



- cubic, space group Fd-3m
- a_{comp} = 5.671 Å
- a_{exp} ≈ 5.658 Å (Ioffe)
- a_{exp} ≈ 5.715 Å (InfoMaticA ave)

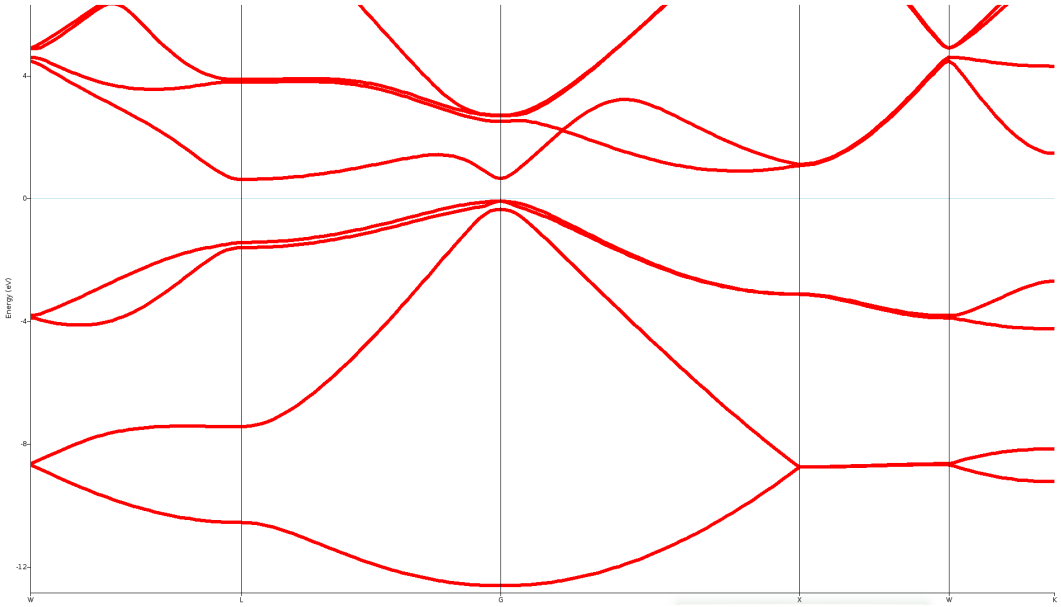


Ioffe: http://www.ioffe.rsi.ru/SVA/NSM/Semicond/

Calculational parameters

- MedeA®-VASP 5.3
- PBEsol functional, spin-orbit relativistic
- standard 500 precision, reciprocal-space projection
- Δ**k** ≈ 0.2/Å, 11×11×11 **k**-points, Γ-centered

Germanium: Electronic Structure



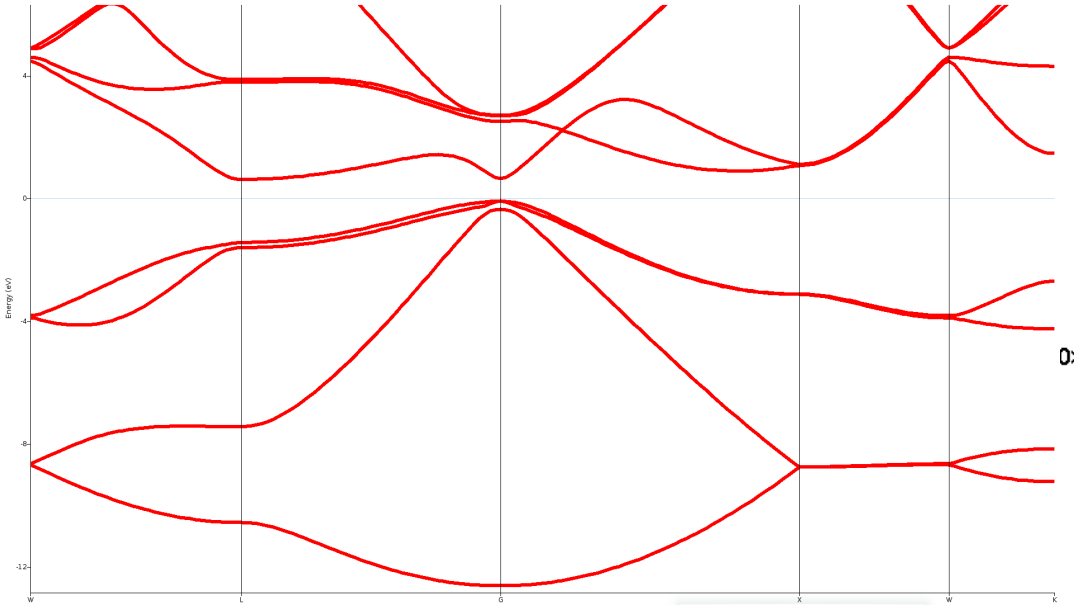
Source	a (Å)	Gap (eV)
mBJLDA	5.658	0.72
mBJLDA	5.671	0.70
Ioffe	5.658 (300K)	0.66 (300K)
Ioffe		0.74 (0K)

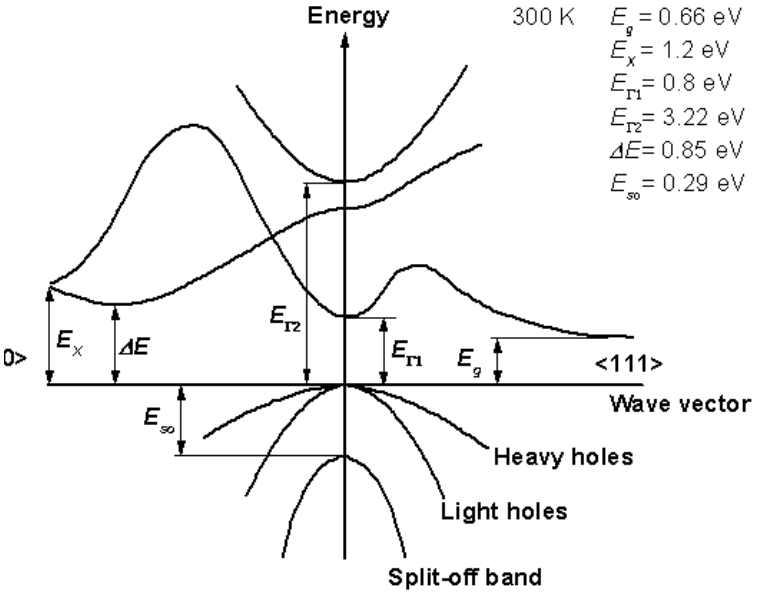
Exp. data: http://www.ioffe.rssi.ru/SVA/NSM/Semicond/
Handbook on Physical Properties of Semiconductors, Vol. 2, ed. S. Adachi (Kluwer, Boston 2004)

Calculational parameters

- MedeA®-VASP 5.3
- mBJLDA functional, spin-orbit relativistic
- normal precision, default plane-wave cutoff
- reciprocal-space projection, linear tetrahedron method
- Δ**k** ≈ 0.2/Å, 11×11×11 **k**-points, Γ-centered

Germanium: Electronic Structure





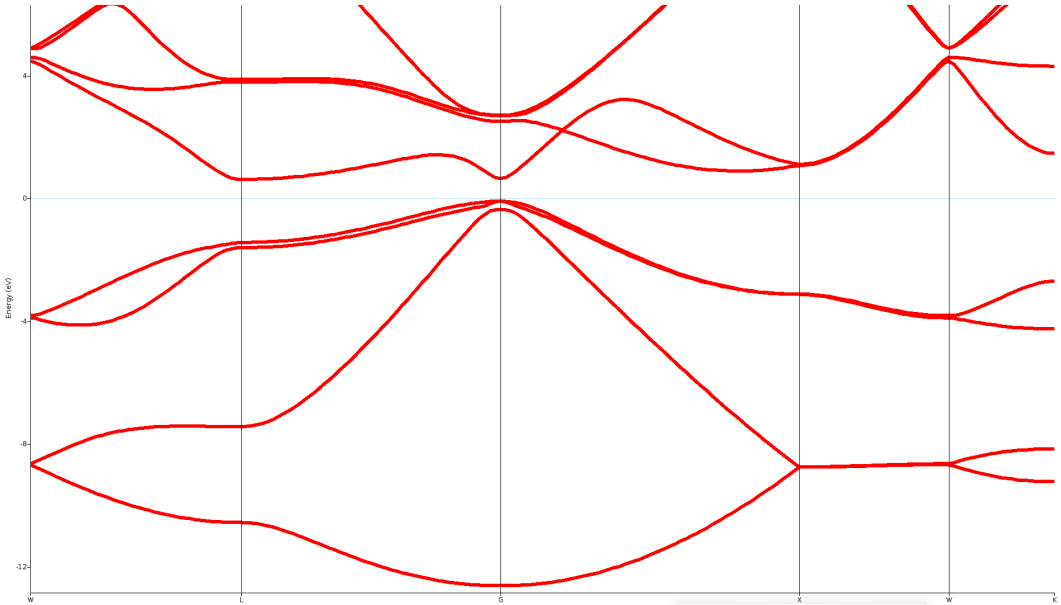
Exp. data: http://www.ioffe.rssi.ru/SVA/NSM/Semicond/

MedeA®-VASP

- computed band energies in good agreement with experimental data
- temperature effects (thermal expansion, phonons) may change the band structure

	Exp.	mBJLDA (5.658)	mBJLDA (5.671)
E_g	0.66	0.72	0.70
ΔE	0.85	0.95	0.98
E_X	1.12	1.15	1.15
E_{SO}	0.29	0.27	0.27
$E_{\Gamma 1}$	0.8	0.80	0.74
$E_{\Gamma 2}$	3.22	2.78	2.78

Germanium: Effective Masses



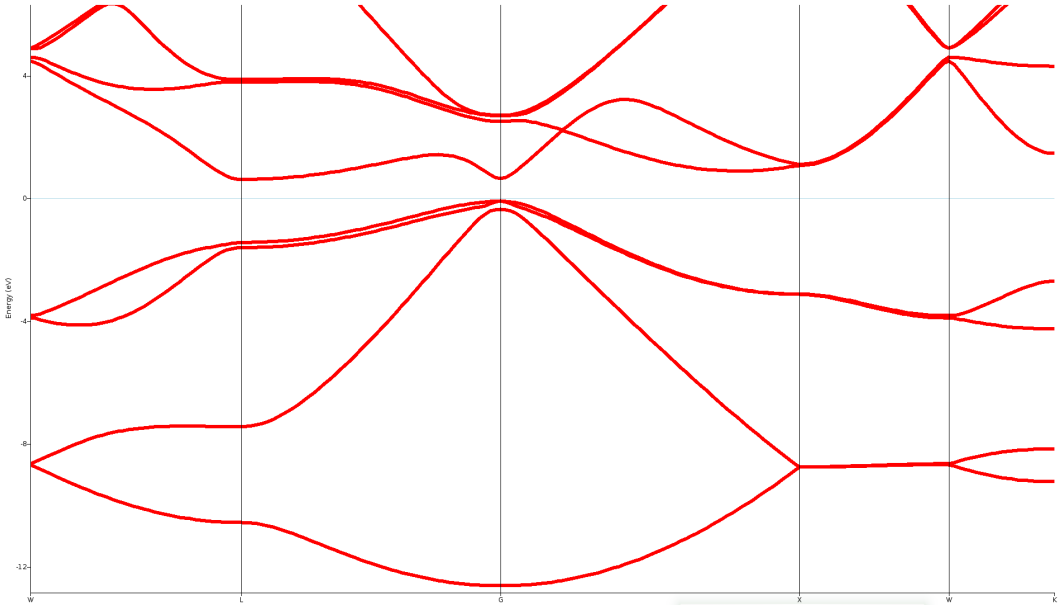
	Exp.	MedeA
Electrons		
Long. Eff. Mass	1.59	1.77
Trans. Eff. Mass	0.081	0.096
DOS Mass	0.22	0.64
Conductivity Mass	0.12	0.14
Heavy Hole		
Eff. Mass	0.33	0.080
Light Hole		
Eff. Mass	0.043	0.085
Split-off band		
Eff. Mass	0.084	0.112

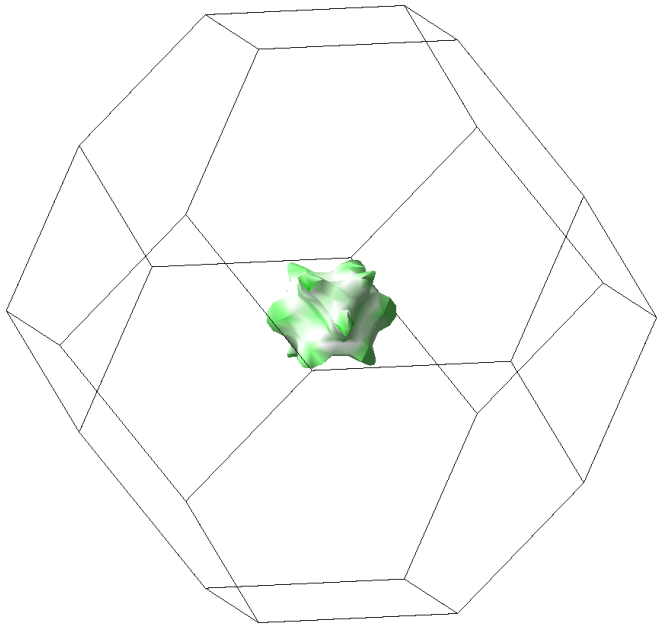
Exp.: http://www.ioffe.rssi.ru/SVA/NSM/Semicond/

MedeA®-Electronics

- computed effective masses in good agreement with experimental data
- heavy hole mass beyond parabolic approximation

Germanium: Effective Masses





MedeA®-Electronics

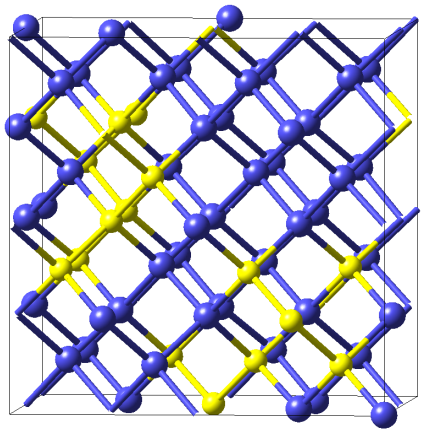
- directional effective masses in reasonable agreement with **k•p** results

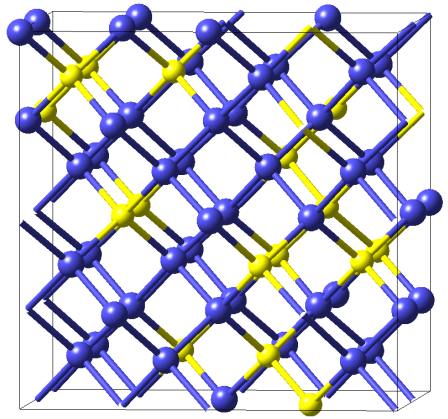
Directional effective masses:

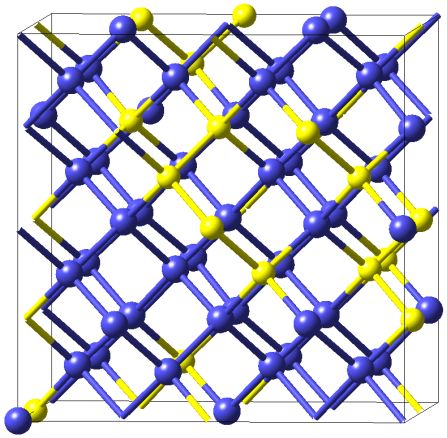
	Heavy Hole			Light Hole		
	Exp.	**k.p**	**calc**	**Exp.**	**k.p**	**calc**
<001>	0.284	0.209	0.111	0.044	0.0459	0.066
<111>	0.376	0.503	0.561	0.043	0.0407	0.0455

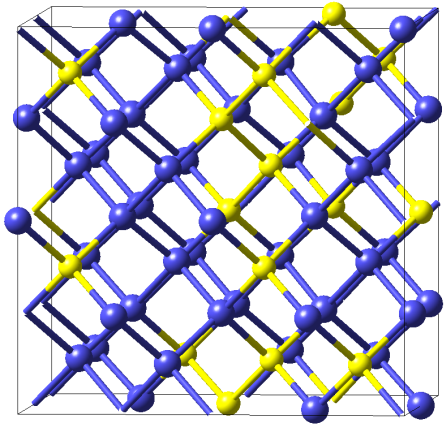
S. Ben Radhia *et al.*, J. Appl. Phys. **92**, 4422 (2002)

$Si_{1-x}Ge_x$: Atomic Structure







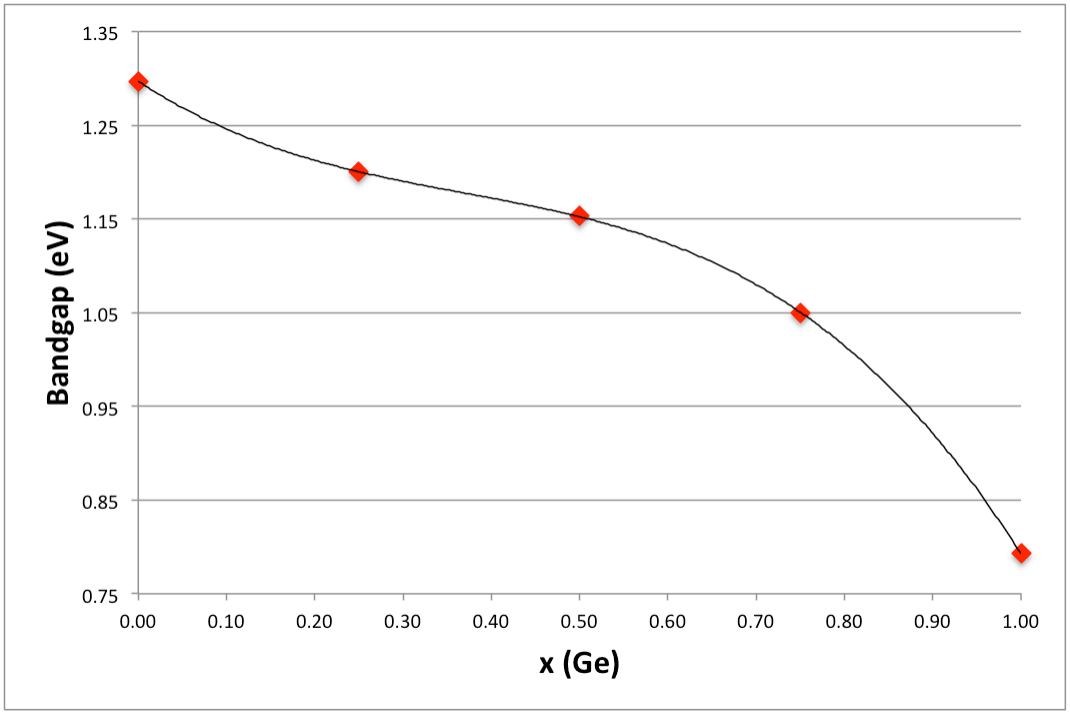


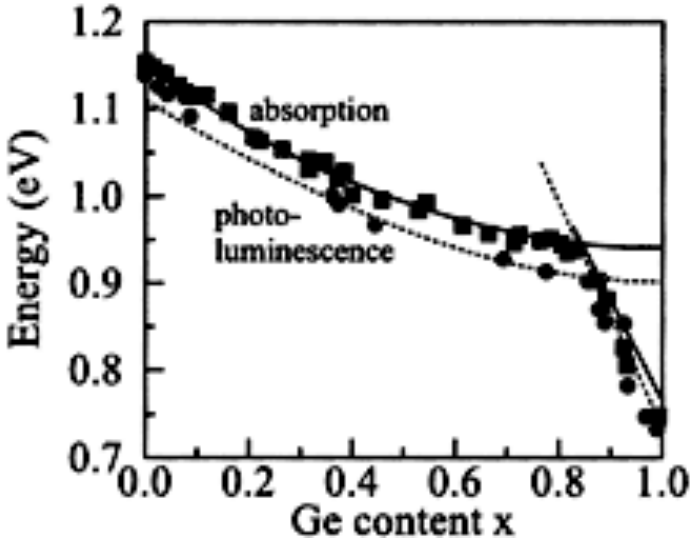
- 2×2×2 supercell of diamond
- replace x×64 Si atoms by Ge
- cubic, space group P1
- relax structure

Calculational parameters

- MedeA®-VASP 5.3
- PBEsol functional
- normal precision, real-space projection
- Δ**k** ≈ 0.2/Å, 3×3×3 **k**-points, Γ-centered

$Si_{1-x}Ge_x$: Electronic Structure





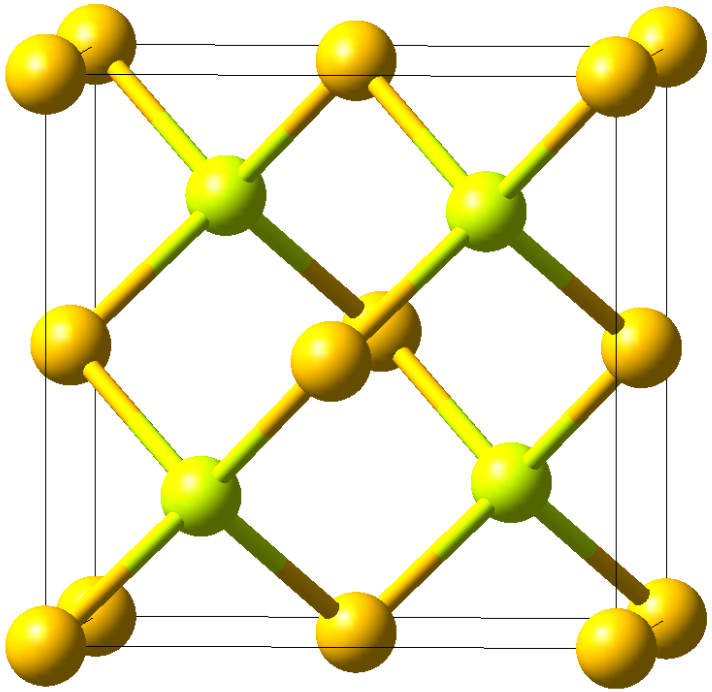
Ioffe: http://www.ioffe.rssi.ru/SVA/NSM/Semicond/

Calculational parameters

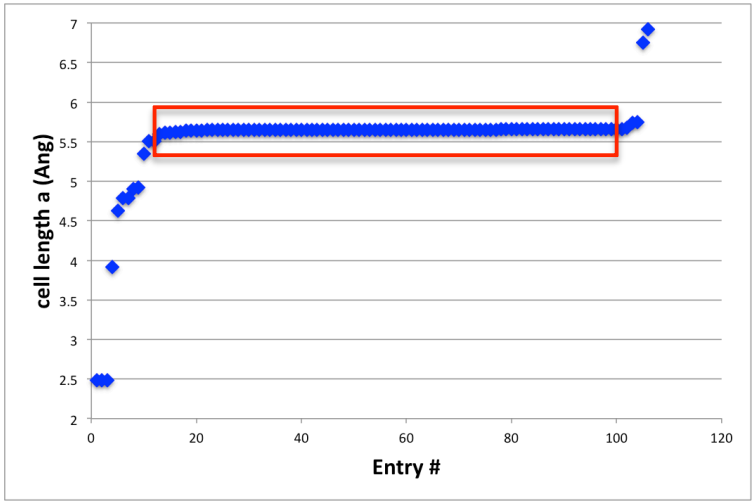
- MedeA®-VASP 5.3
- mBJLDA functional
- normal precision, real-space projection
- Δ**k** ≈ 0.2/Å, 3×3×3 **k**-points, Γ-centered

- calculations give band gap trend in close agreement with experimental data
- band gap variation due to disorder ≈ 0.05 eV
- band gap is slightly over-estimated

GaAs: Atomic Structure



- cubic, space group F-43m
- a_{comp} = 5.671 Å
- a_{exp} ≈ 5.65325 Å (Ioffe)
- a_{exp} ≈ 5.6477 Å (InfoMaticA ave)

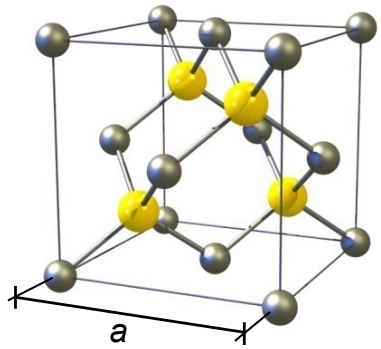


Ioffe: http://www.ioffe.rssi.ru/SVA/NSM/Semicond/

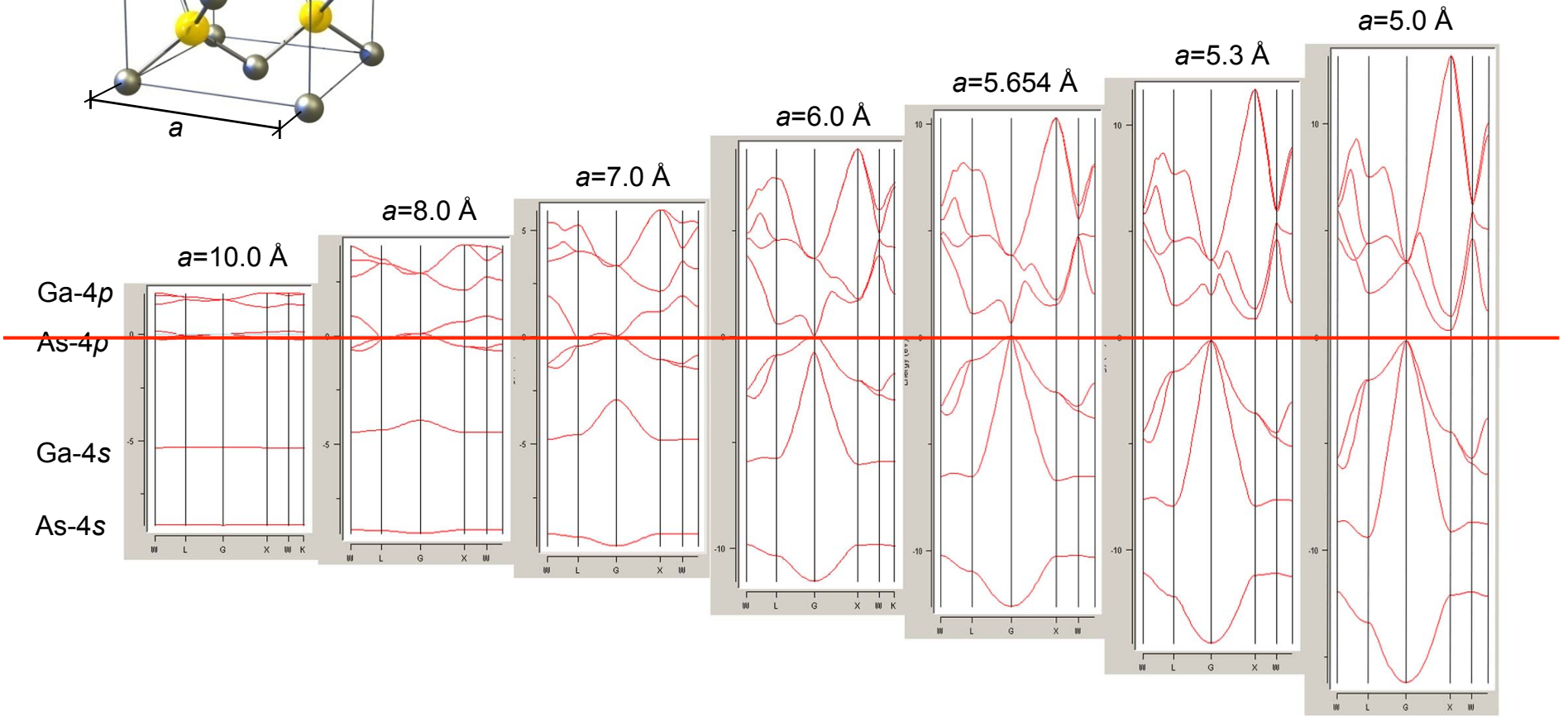
Calculational parameters:

- MedeA®-VASP 5.3
- PBEsol functional, spin-orbit relativistic
- standard 500 precision, reciprocal-space projection
- Δ**k** ≈ 0.2/Å, 11×11×11 **k**-points, Γ-centered

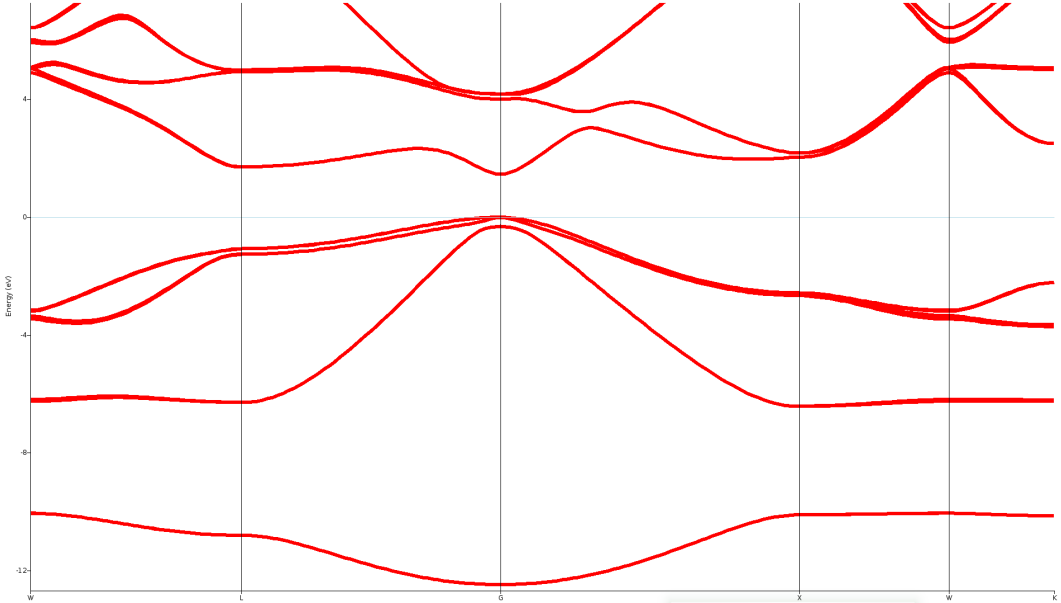
GaAs: Electronic Bands vs. Volume



GaAs



GaAs: Electronic Structure



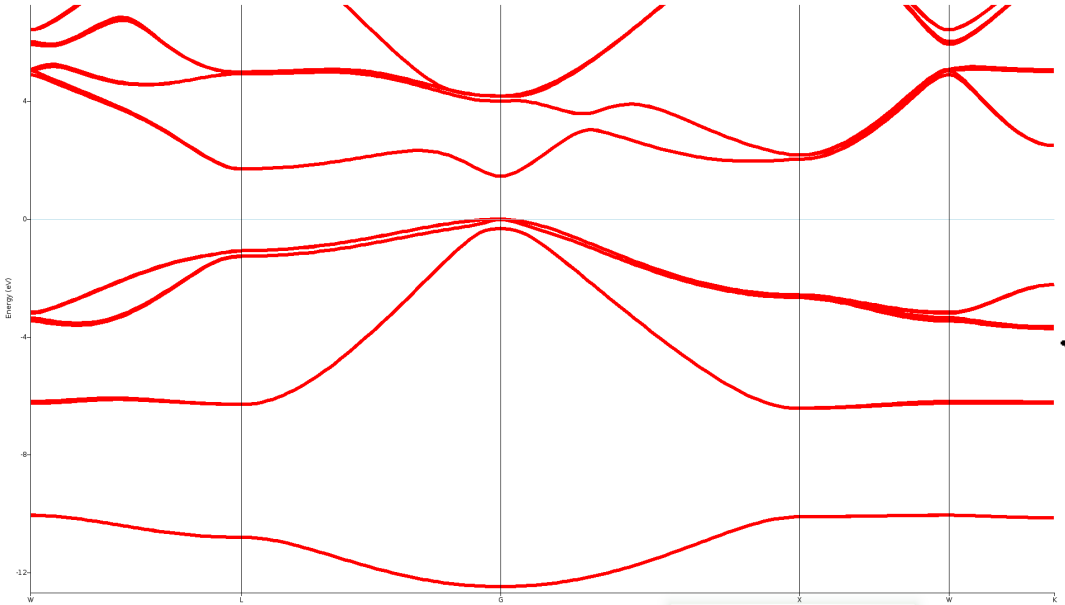
Source	a (Å)	Gap (eV)
mBJLDA	5.653	1.510
mBJLDA	5.671	1.472
Ioffe	5.653 (300K)	1.424 (300K)
Ioffe		1.519 (0K)
Handbook	5.653 (300K)	1.43 (300K)
Handbook		1.52 (0K)

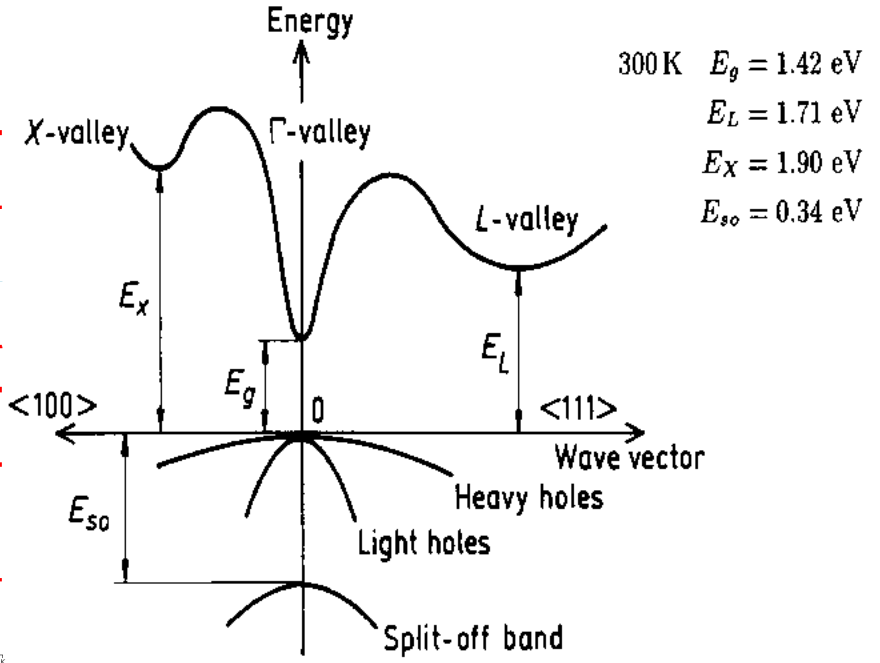
Exp. data: http://www.ioffe.rssi.ru/SVA/NSM/Semicond/
Handbook on Physical Properties of Semiconductors, Vol. 2, ed. S. Adachi (Kluwer, Boston 2004)

Calculational Parameters

- MedeA®-VASP 5.3
- mBJLDA functional, spin-orbit relativistic
- normal precision, default plane-wave cutoff
- reciprocal-space projection, linear tetrahedron method
- Δ**k** ≈ 0.2/Å, 11×11×11 **k**-points, Γ-centered

GaAs: Electronic Structure





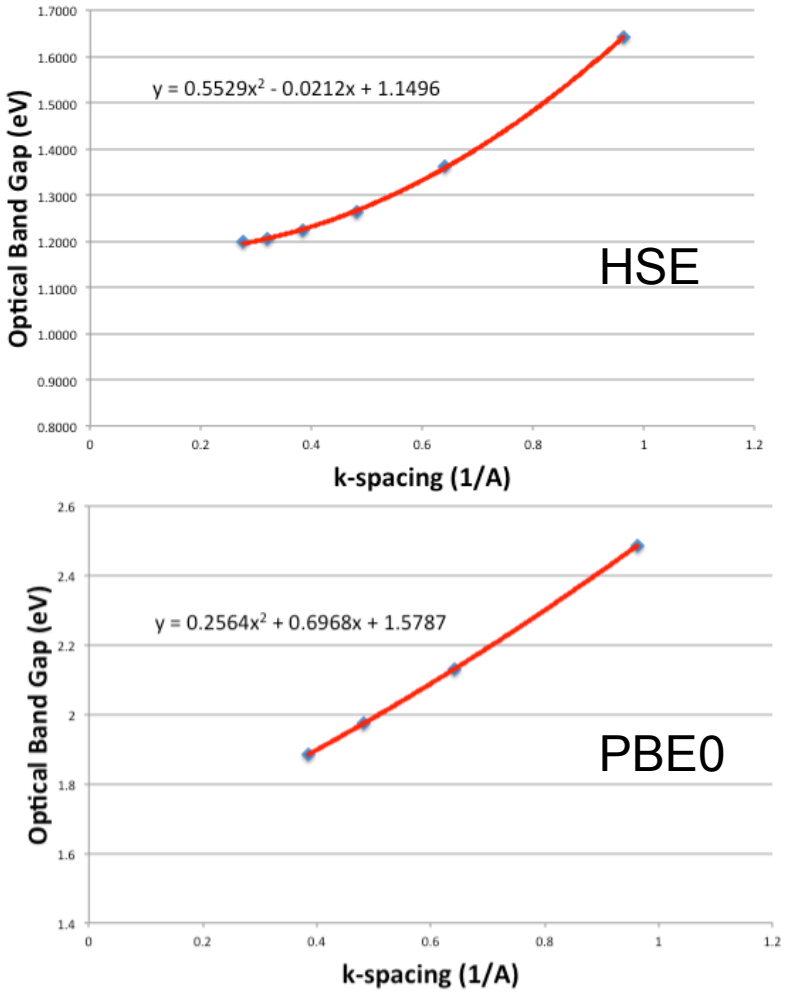
Exp. data: http://www.ioffe.rssi.ru/SVA/NSM/Semicond/
Handbook on Physical Properties of Semiconductors, Vol. 2, ed. S. Adachi (Kluwer, Boston 2004)

MedeA®-VASP

- computed band energies in good agreement with experimental data
- temperature effects (thermal expansion, phonons) may induce changes (≈ 0.1 eV)

	Exp. (0 K)	Exp. (300 K)	mBJLDA (5.653)	mBJLDA (5.671)
E_g	1.52	1.42	1.50	1.47
E_L	1.78	1.71	1.73	1.70
E_X	2.00	1.90	1.96	1.96
E_{SO}	0.34	0.34	0.31	0.31

GaAs: Electronic Structure



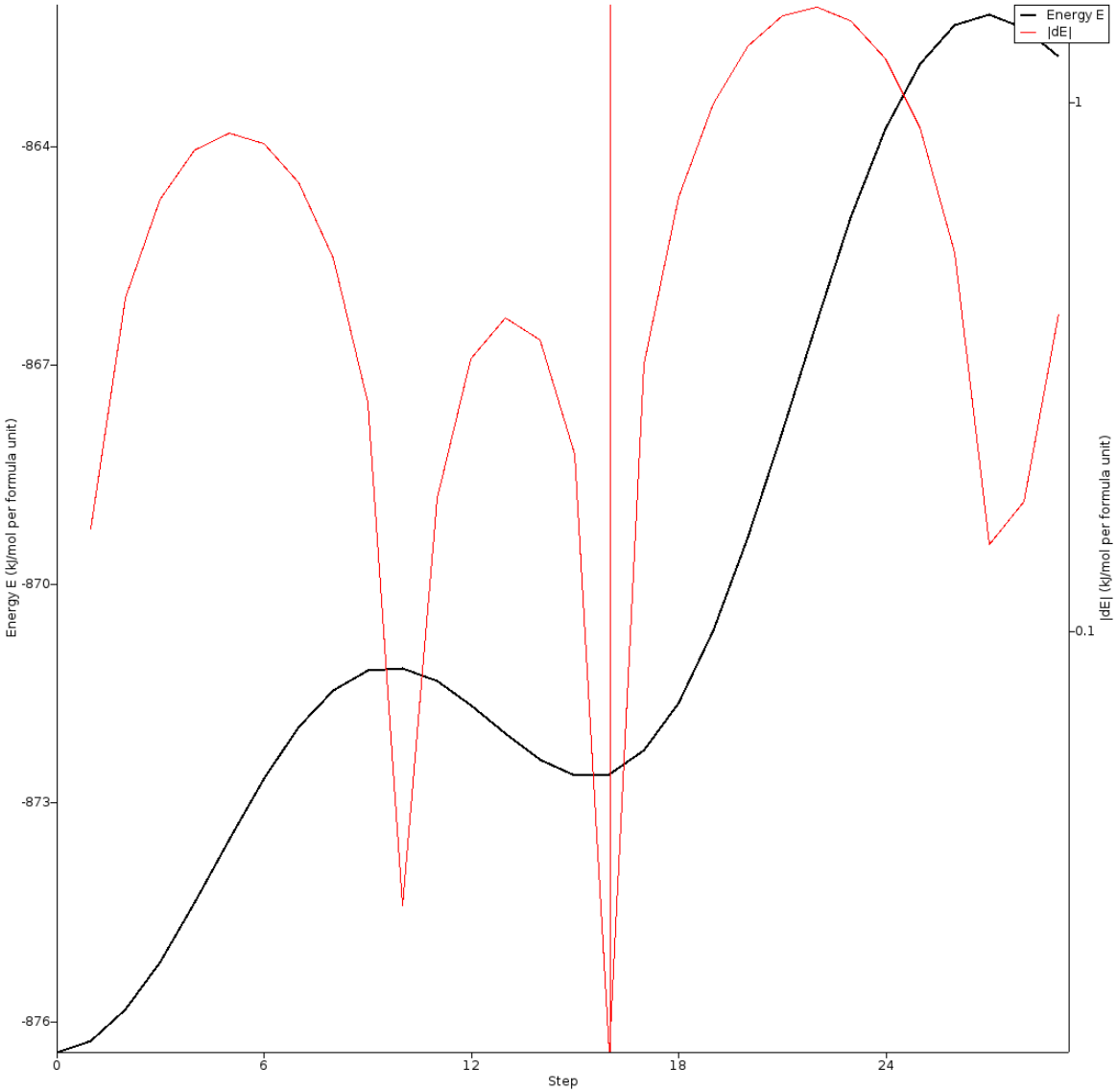
- Γ-centered meshes
- identical for scf and nIX

Source	a (Å)	Gap (eV)
HSE	5.655	1.15
PBE0	5.655	1.579
Ioffe	5.653 (300K)	1.424 (300K)
Ioffe		1.519 (0K)
Handbook	5.653 (300K)	1.43 (300K)
Handbook		1.52 (0K)

Exp. data: http://www.ioffe.rssi.ru/SVA/NSM/Semicond/
Handbook on Physical Properties of Semiconductors, Vol. 2, ed. S. Adachi (Kluwer, Boston 2004)

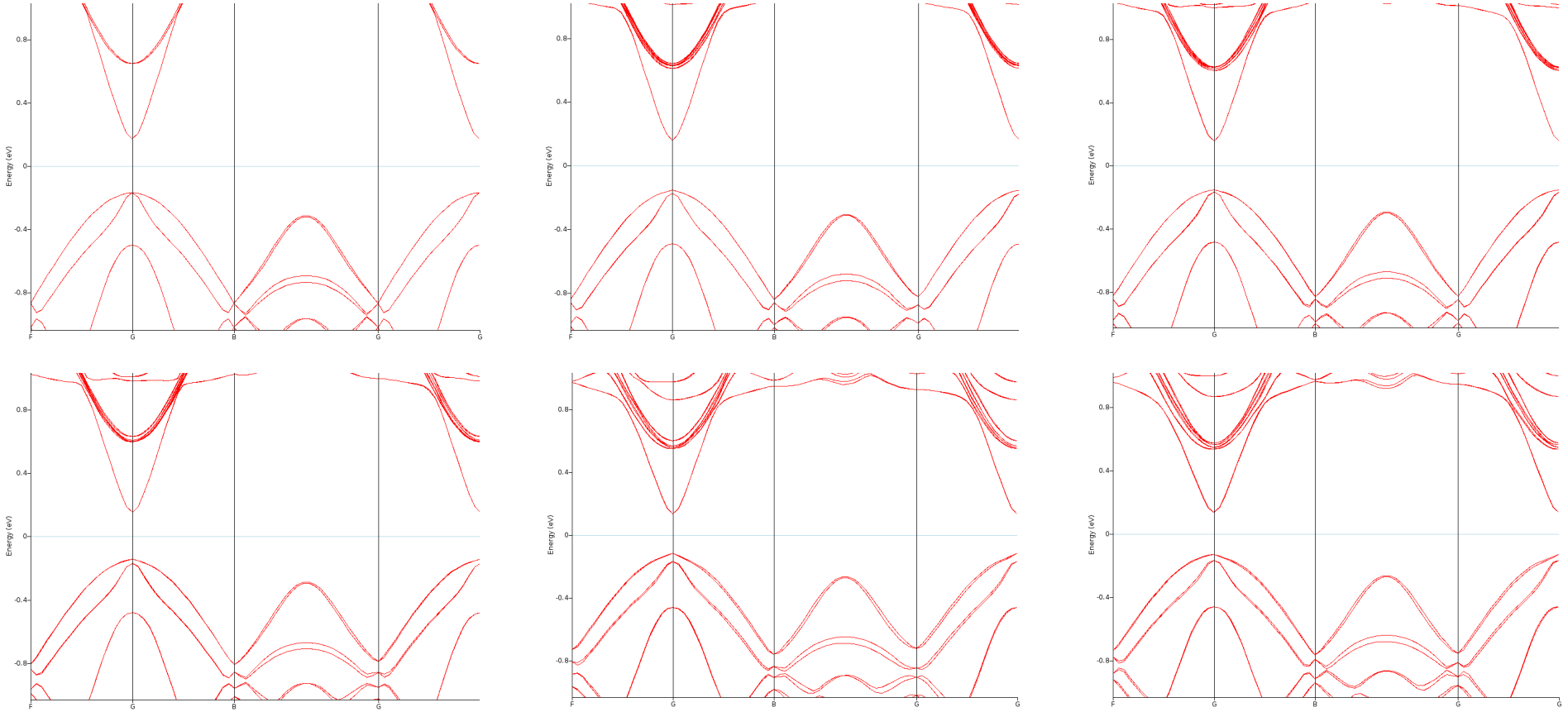
- HSE underestimates E_{gap}
- E_{gap} depends on lattice constant!
- E_{gap} hardly depends on accuracy, pw-cutoff, # bands
- E_{gap} determined by smaller of scf and nIX **k**-spacing

GaAs: MD Simulations



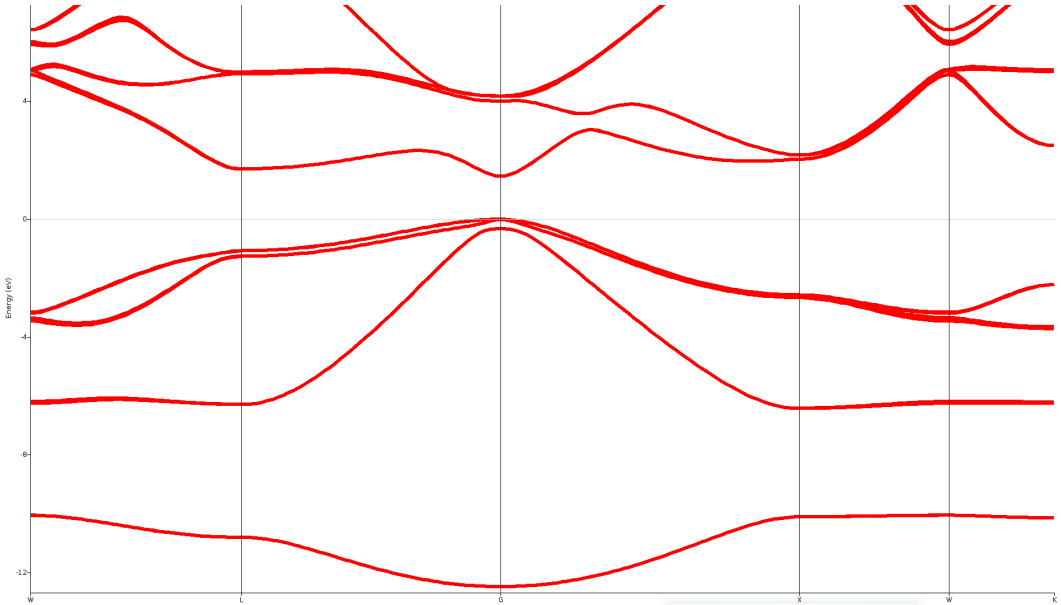
- Ab initio MD at 298 K
- 2×2×2 supercell
- MedeA®-VASP 5.3
- PBEsol functional
- SO coupling
- normal precision
- PW cutoff 282.691 eV
- real-space projection
- Γ-centered mesh with 0.3/Å **k**-point spacing, i.e. 2×2×2 **k**-points

GaAs: MD Simulations



- band gap varies by ≈ 0.1 eV
- HH-LH and HH-SO splittings vary by ≈ 0.05 eV
- different splittings of 2nd conduction band

GaAs: Effective Masses



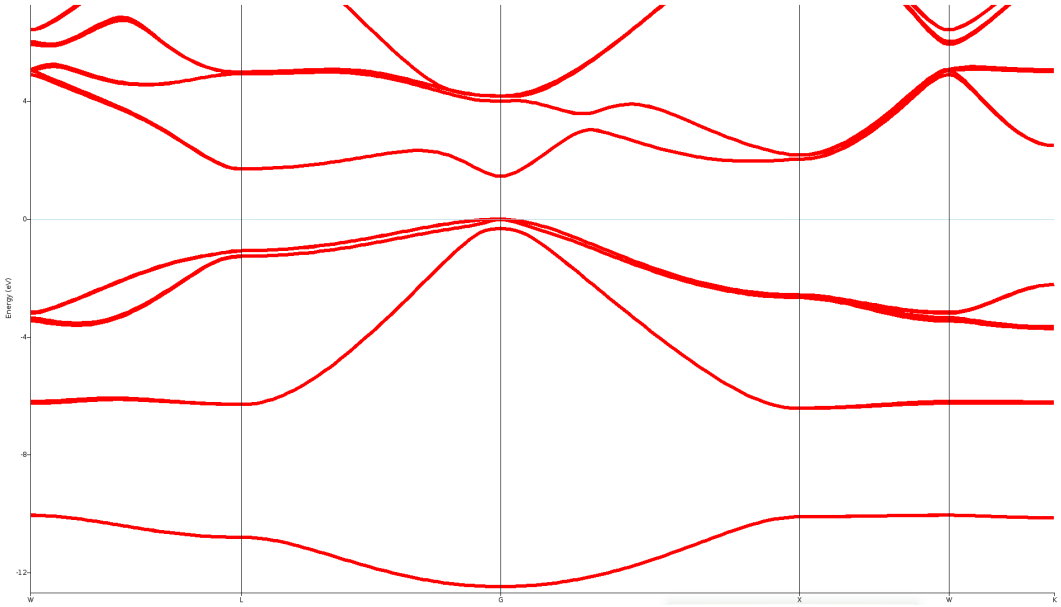
	Exp.	Exp.	MedeA
Electrons			
Eff. Mass @Γ	0.063	0.064	0.088
Long. Eff. Mass @L	1.9	1.9	1.16
Trans. Eff. Mass @L	0.075	0.075	0.19
Long. Eff. Mass @X	1.9	1.3	1.01
Trans. Eff. Mass @x	0.19	0.23	0.20
Heavy Hole			
Eff. Mass	0.51	0.50	0.64/0.73
Light Hole			
Eff. Mass	0.082	0.082	0.098
Split-off band			
Eff. Mass	0.15	0.15-0.18	0.206

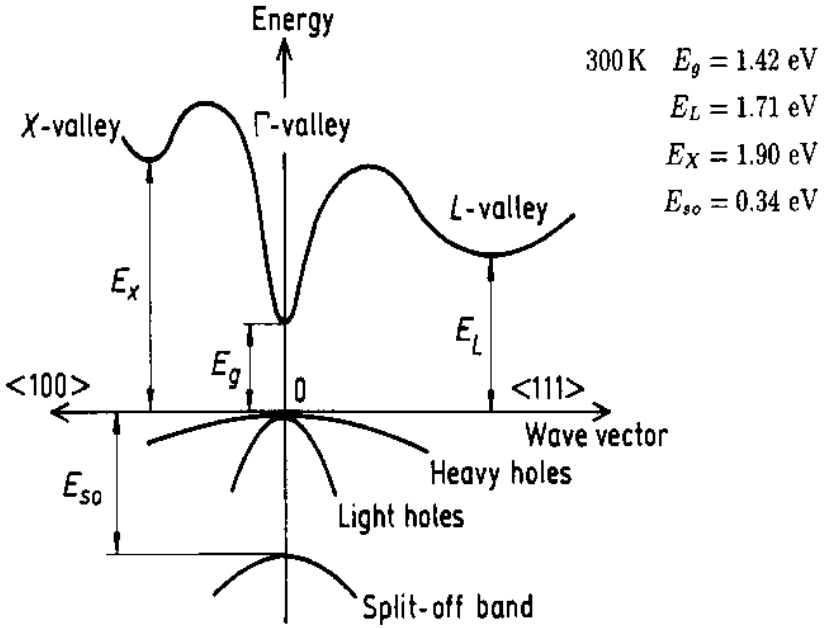
Exp. data: http://www.ioffe.rssi.ru/SVA/NSM/Semicond/
Handbook on Physical Properties of Semiconductors, Vol. 2, ed. S. Adachi (Kluwer, Boston 2004)

MedeA®-Electronics

- computed effective masses in good agreement with experimental data
- heavy hole mass beyond parabolic approximation

GaAs: Effective Masses





Exp. data: http://www.ioffe.rssi.ru/SVA/NSM/Semicond/
Handbook on Physical Properties of Semiconductors, Vol. 2, ed. S. Adachi (Kluwer, Boston 2004)

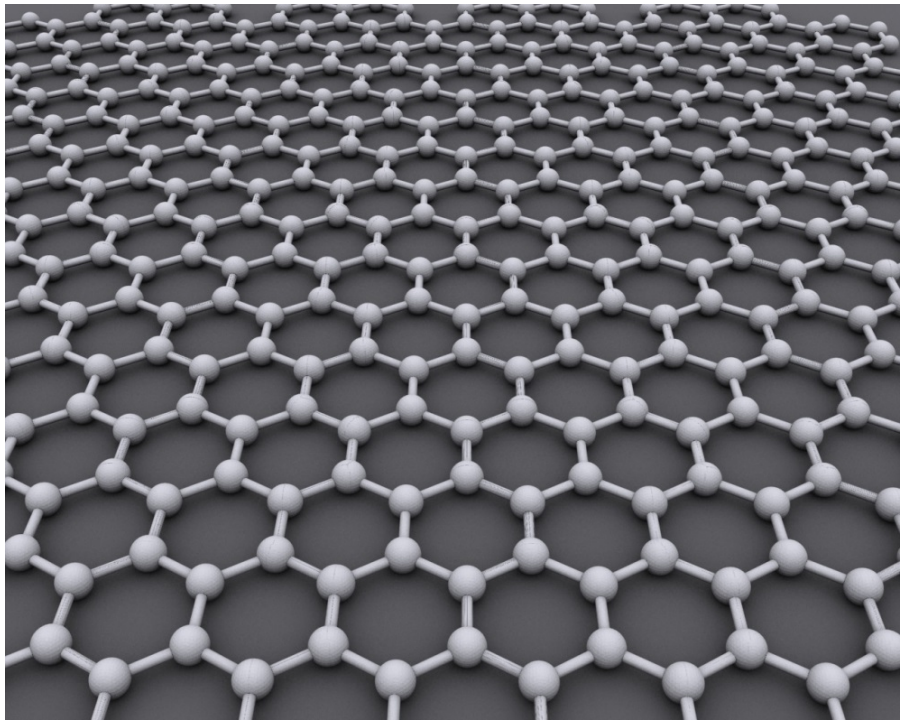
MedeA®-Electronics

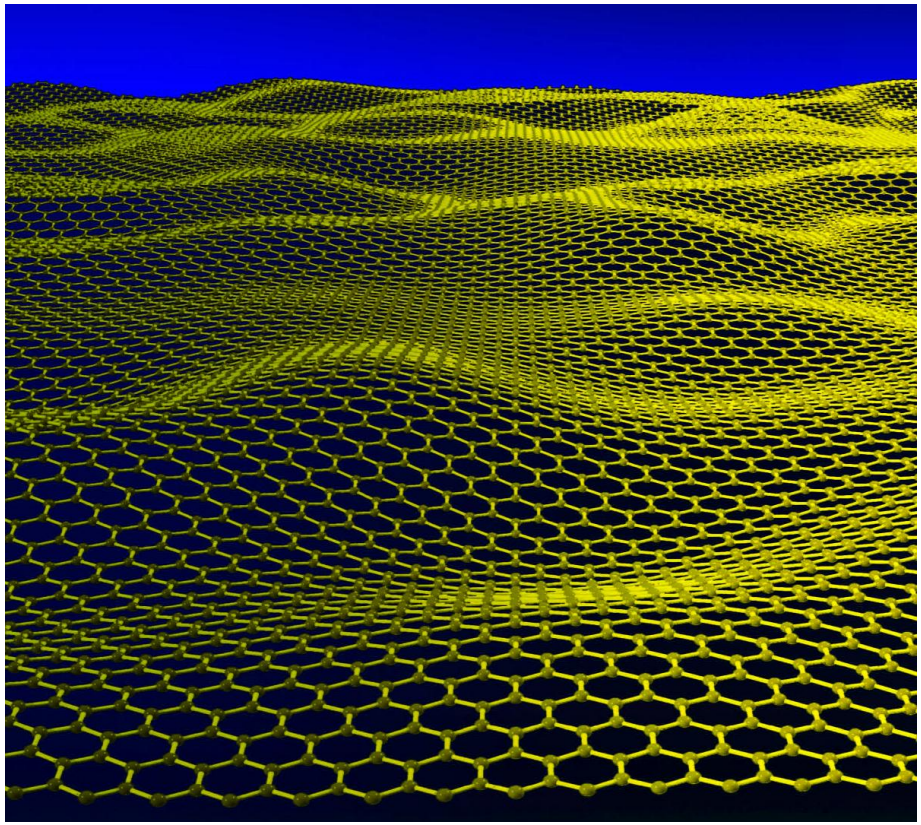
- directional effective masses in reasonable agreement with experimental data

	Heavy Hole		Light Hole		Split-Off	
	Exp.	calc	Exp.	calc	Exp.	calc
<001>	0.330	0.314	0.090	0.099	0.154 - 0.178	0.207
<011>		2.949		0.089		0.208
<111>	0.780	2.838	0.077	0.084		0.205

Phonon Dispersions

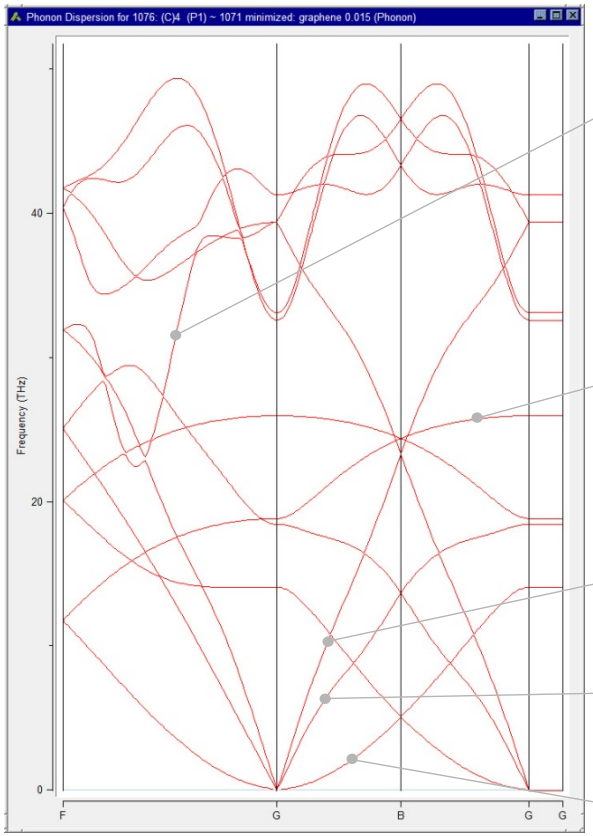
Graphene

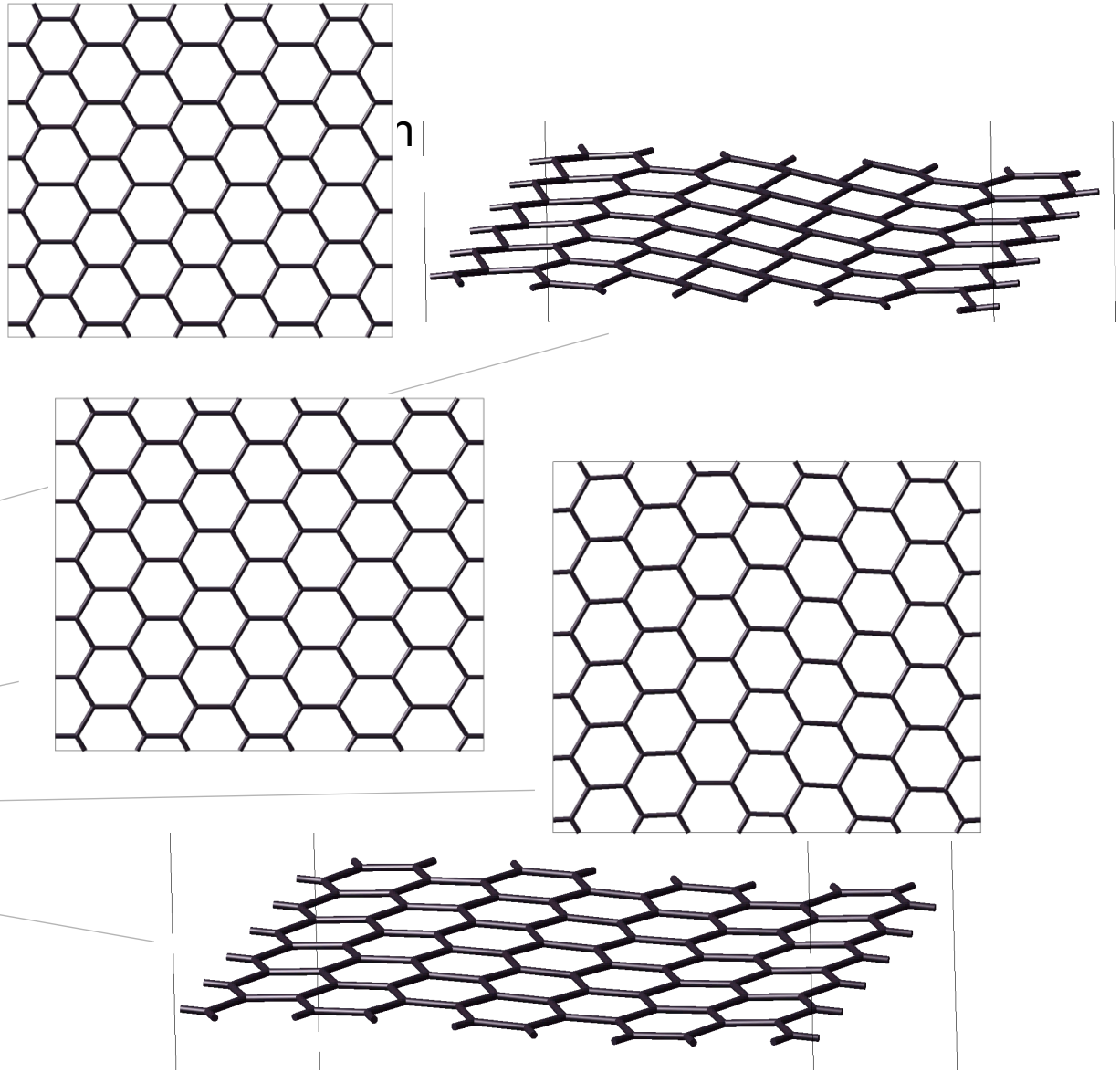




- Konstantin Novoselov, Andre Geim
  - first isolated individual graphene planes in 2004
  - nobel prize 2010

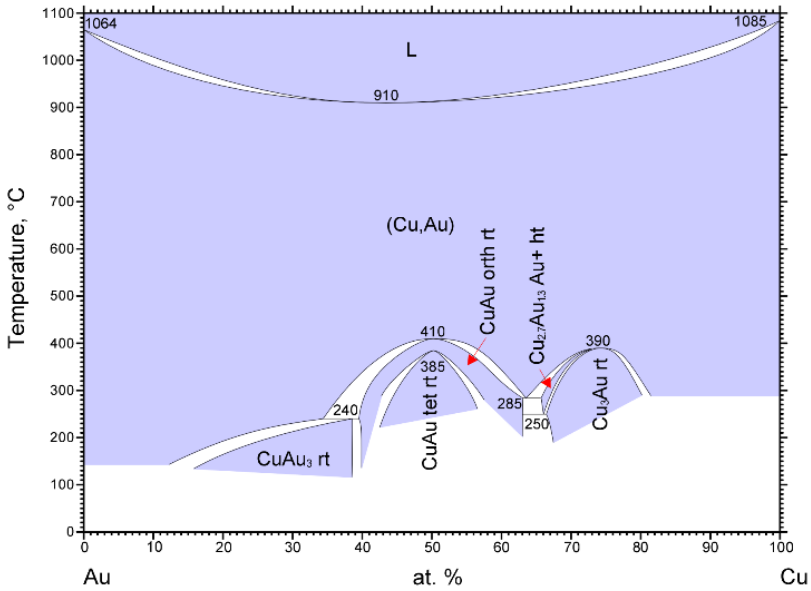
Analyze Phonons of Graphene





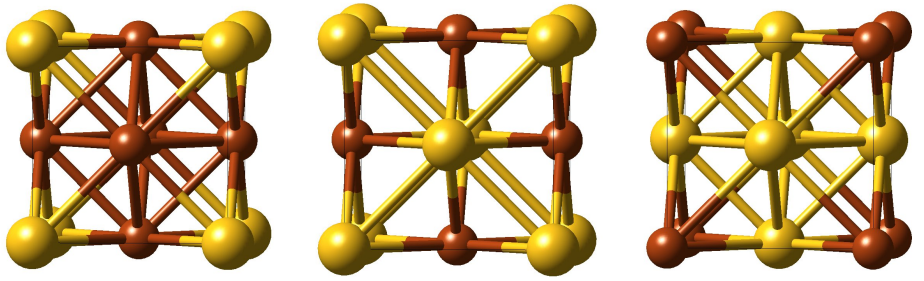
Electrical Conductivity in Disordered Materials

$Cu_{1-x}Au_x$: Intermetallic Phases

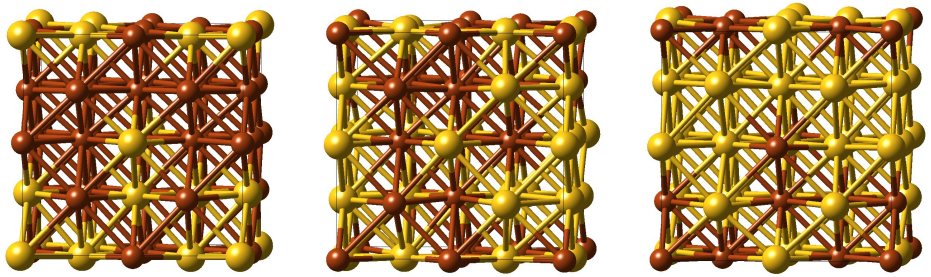


- wide range of solubility
- ordered and disordered phases

ordered cubic phases (InfoMaticA):



disordered cubic phases (SQS):

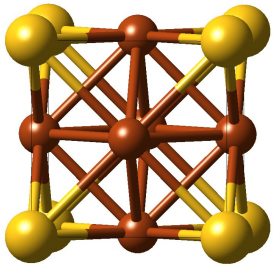


Cu_3Au $CuAu$ $CuAu_3$

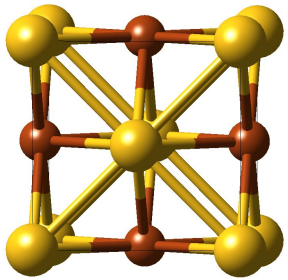
- ordered phases from literature (InfomaticA) and cluster expansion (CE)
- disordered phases modeled as quasi-random structure (SQS)
  - mimic first few correlation functions of perfectly random structures

$Cu_{1-x}Au_x$: Ordered Structures

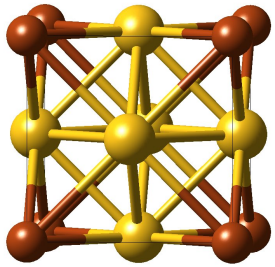
ordered cubic phases (InfoMaticA):



Cu_3Au

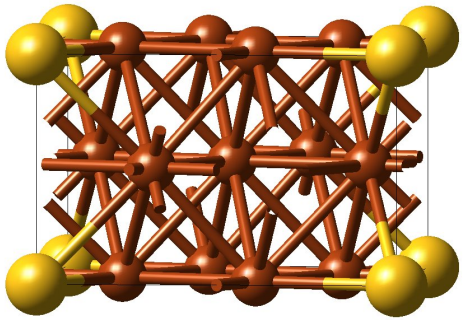


$CuAu$

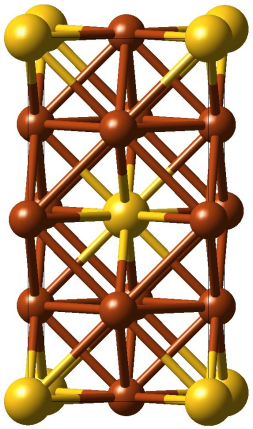


$CuAu_3$

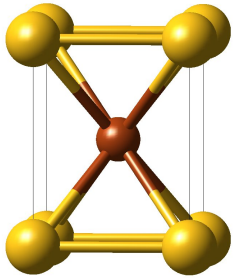
ordered tetragonal phases from cluster expansion (CE):



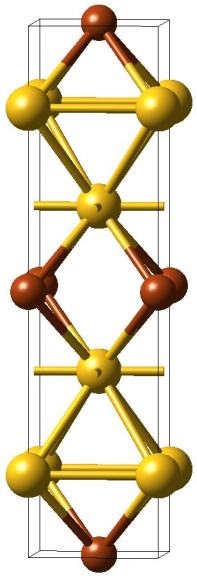
Cu_9Au



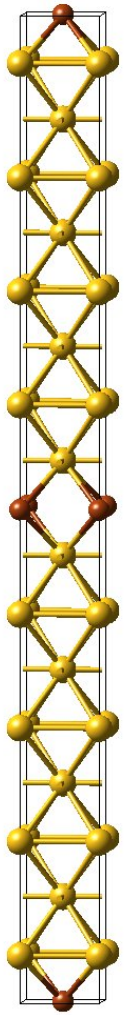
Cu_3Au



$CuAu$



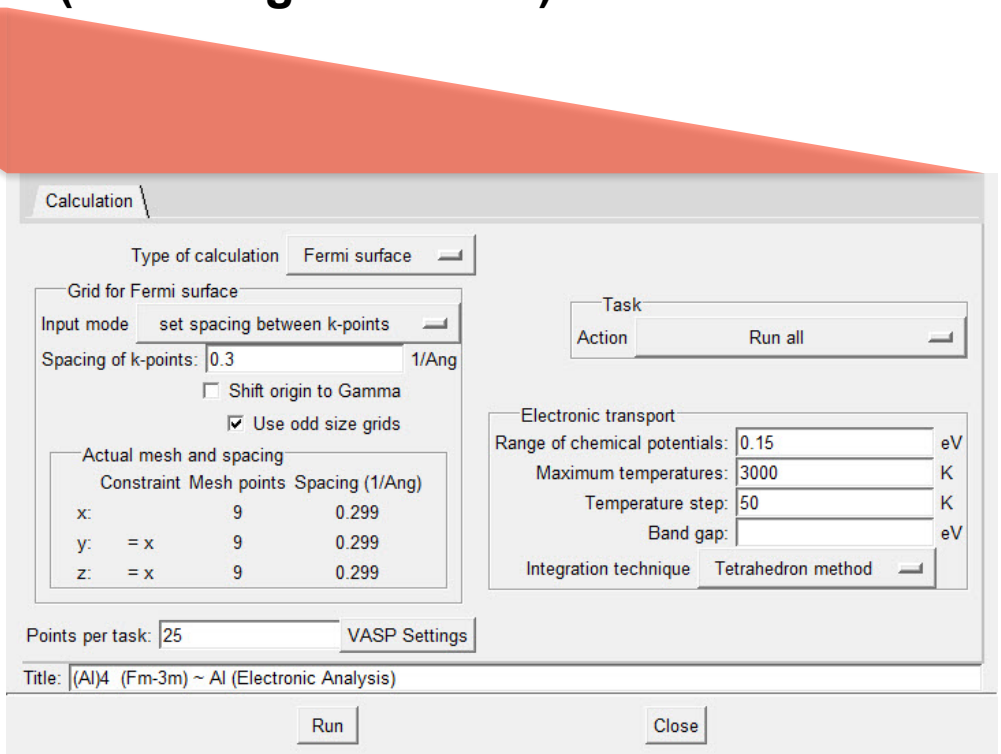
$CuAu_2$



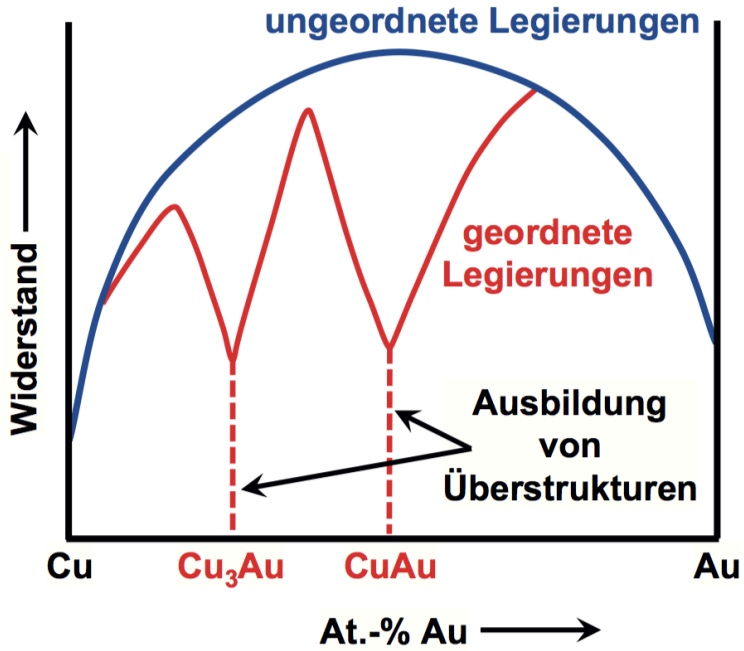
$CuAu_8$

MedeA® Electronics

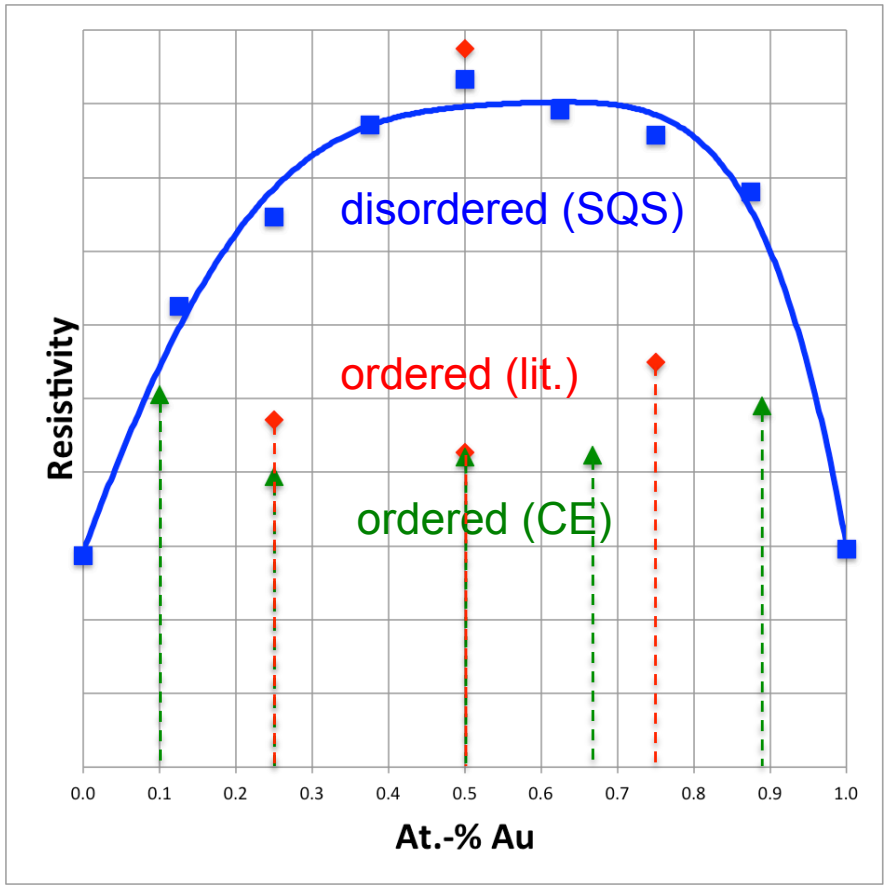
- Boltzmann theory: semiclassical theory
  - electrons follow classical equations of motion
  - electron velocity/effective mass from first principles
  - results depend on relaxation time (**critical!**)
- implemented in **MedeA® Electronics (including BoltzTraP)**
- calculated properties
  - electrical conductivity
  - thermopower (Seebeck coefficient)
  - thermal conductivity (electronic part)
  - electronic specific heat
  - Pauli paramagnetic susceptibility
  - Hall conductivity
- results vs. temperature or doping



$Cu_{1-x}Au_x$: Electrical Resistivities



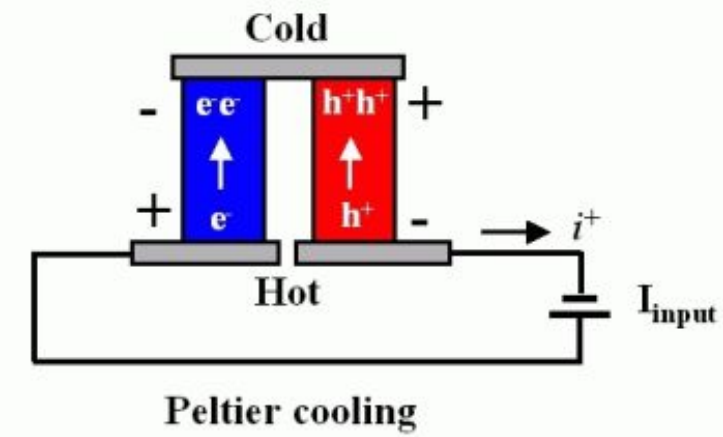
Pecher, Haarmann, Nachr. Chem. **61**, 1017 (2013);
Riedel, Janiak, *Anorg. Chem.* (de Gruyter, Berlin 2007)

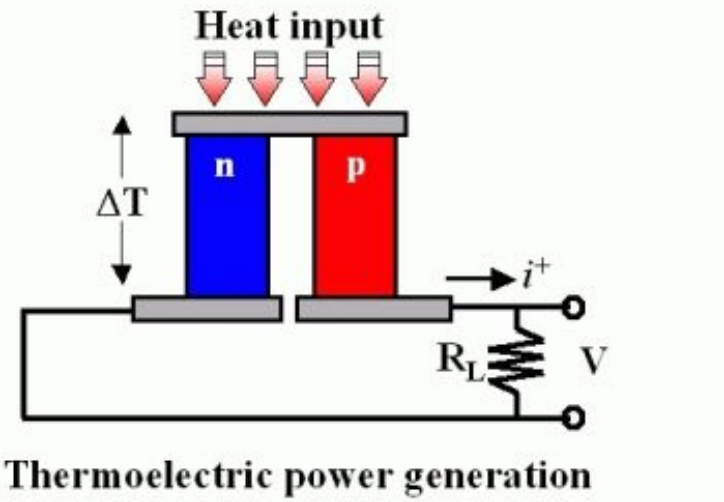


- ordered phases show systematically reduced electrical resistivities as compared to disordered alloys
- very good agreement of calculated data with experimental findings

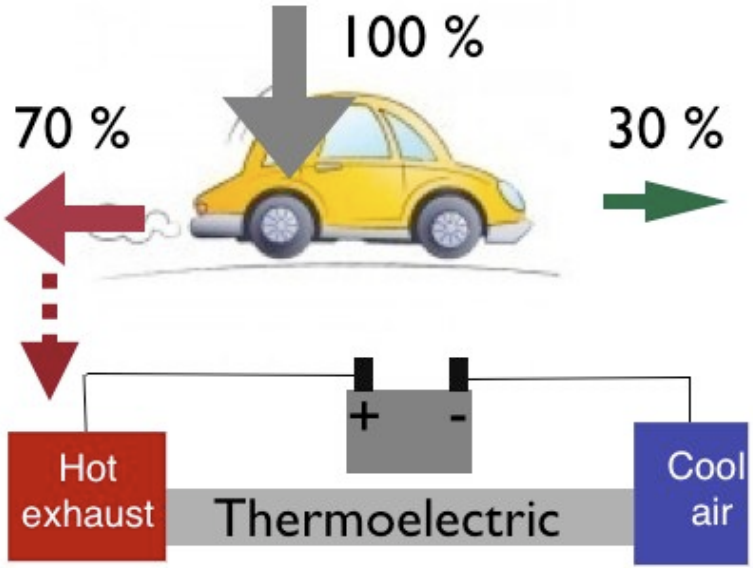
Thermoelectric Power of Bi_2Te_3

Thermoelectricity





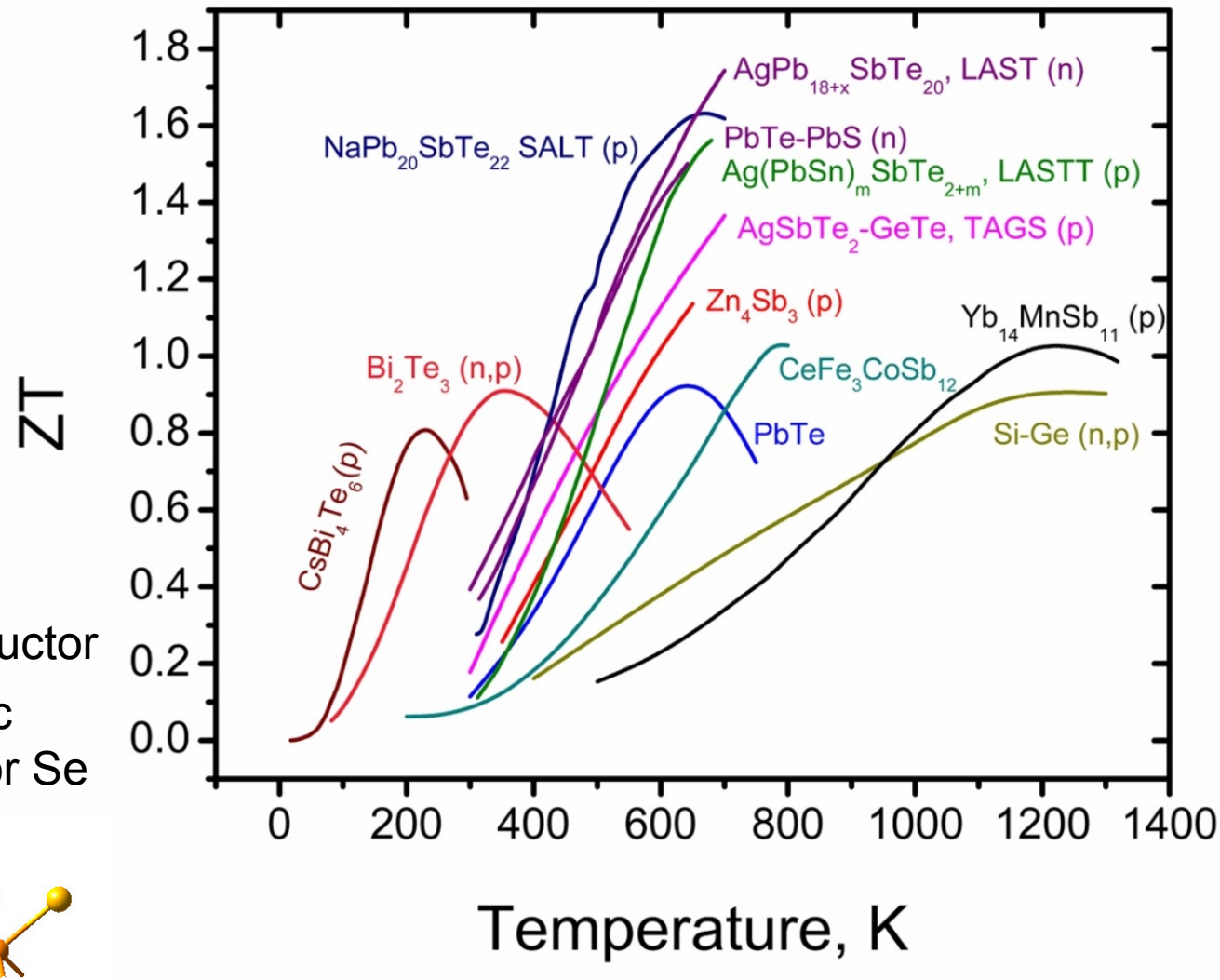
- Peltier effect
  - use electric power for heating or cooling
- Seebeck effect
  - convert heat into electric power



Promising Candidates

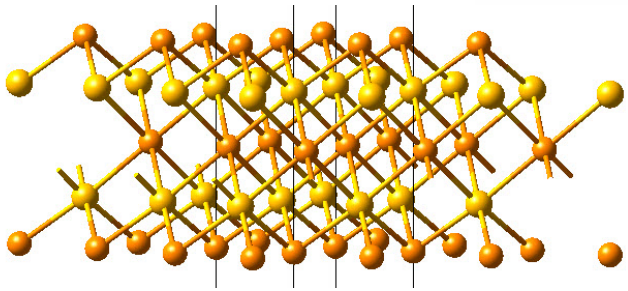
Figure of merit:

$$Z = \sigma S^2/\kappa$$



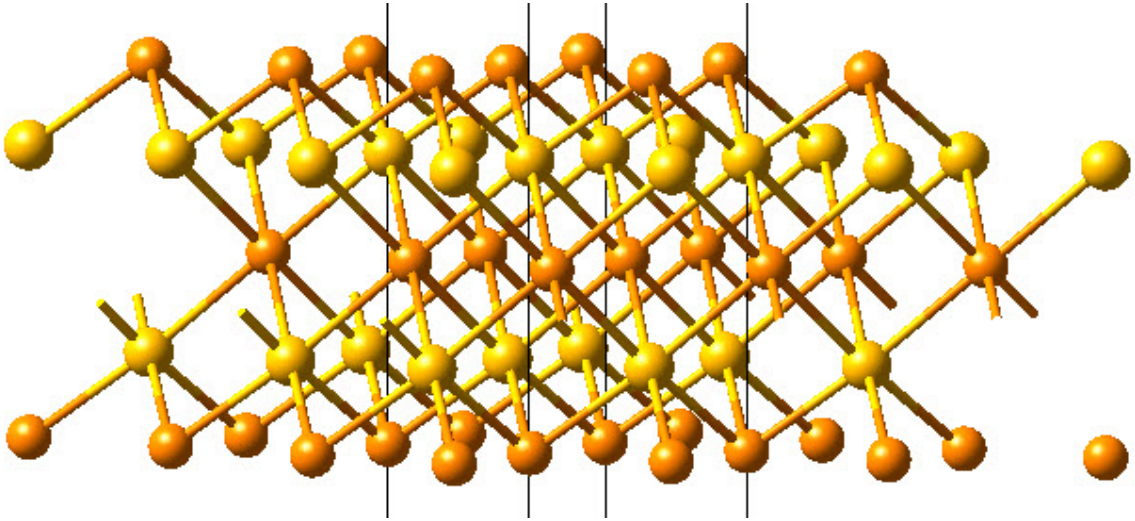
Bi_2Te_3

- layered structure
- narrow-gap semiconductor
- efficient thermoelectric when doped with Sb or Se



Retrieve structure of Bi_2Te_3

- ***Tools*** → ***InfoMaticA***, ***InfoMaticA*** → ***Search, Clear***
- Define the search criteria
  - **Formula is** ***Bi2Te3***
  - **Structural completeness** is ***Complete***
- Retrieve the relevant crystal structures of Bi_2Te_3
  - Select structures *ICSD.42546* (hexagonal setting of rhombohedral phase)
  - ***Right-click*** on one selected record → ***View***
  - Draw bonds: ***Right-click*** in the structure window → ***Edit bonds…***, ***OK***

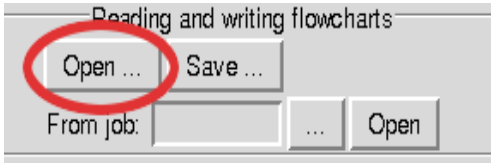


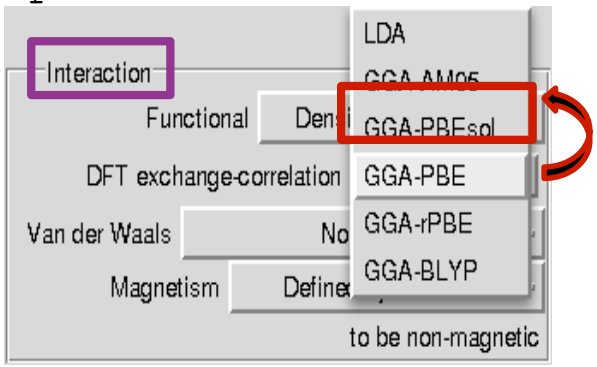
layered rhombohedral structure

- covalent bonding within slabs
- van der Waals bonding between slabs

Optimize Structure

- Activate Bi_2Te_3 structure
- ***Job Control*** → ***New Job…***
  - ***Right-click*** on left area → ***Clear***
  - **Open …** → Load the flowchart `Bi2Te3-full-optimization.flow` from the training flowchart folder
  - ***Right-click*** on VASP stage → ***Edit…***
  - Change DFT exchange-correlation to **GGA-PBEsol**
  - **Ok**
  - Enter as **Job title:** Bi2Te3 full optimization PBEsol+SOI
  - ***Run***

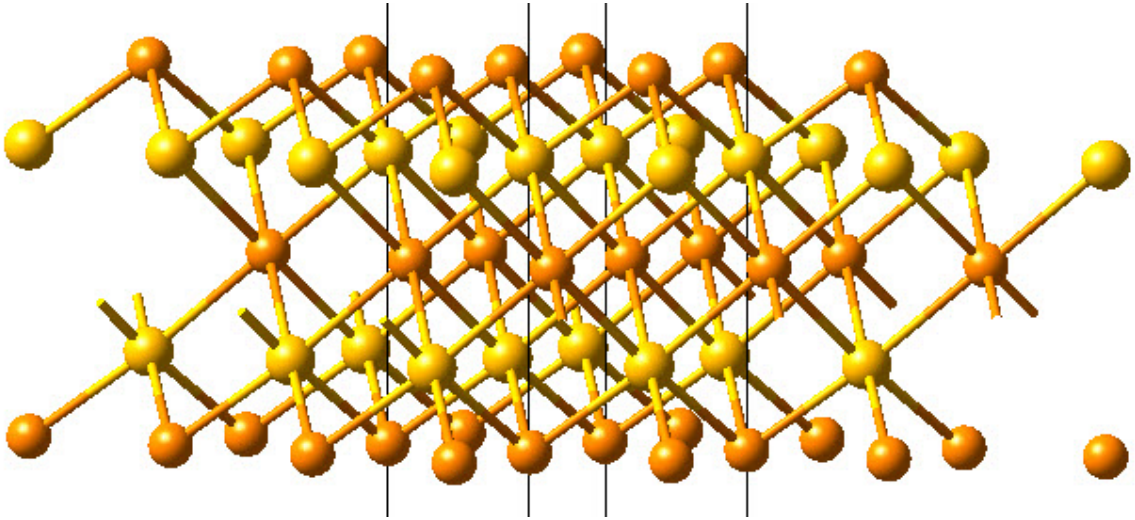




(Only set up the VASP jobs but do not actually run them!)

Monitor and load optimized structure

- Clear MedeA® workbench: ***Windows*** → ***Close all windows***
- Check and analyse results:
  - ***Job Control*** → ***View and Control Jobs*** (opens JobServer interface in web browser)
  - Click on Jobs and afterwards on relevant job number of the running jobs
  - Check the progress of the calculation (indicated by **Available Results**)
- Upon completion of jobs load the optimized structures
  - ***File*** → ***Open…*** → ***Previous Calculation***
  - Select the `final:` record of the relevant job
  - ***Insert >>***, ***Ok***

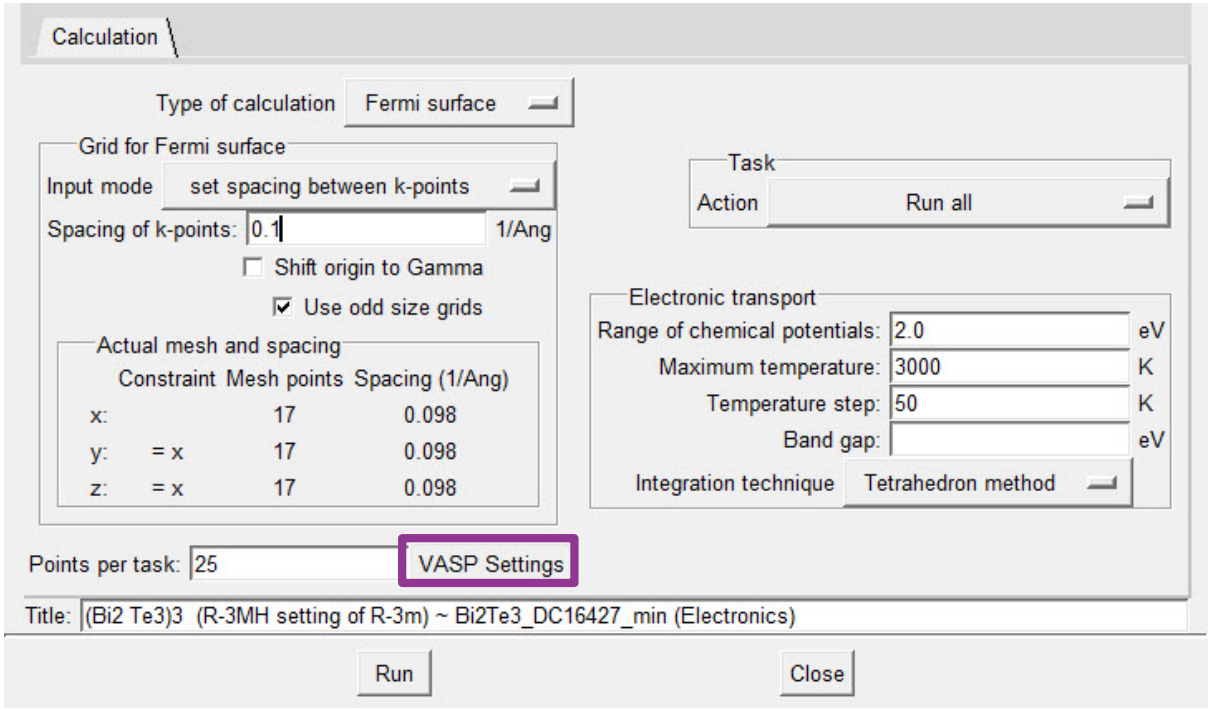


layered rhombohedral structure

- covalent bonding within slabs
- van der Waals bonding between slabs

Set up MedeA® Electronics job

- Activate the optimized tetragonal structure
- Open Electronics module: **Tools** → **Electronics**, **Electronics** → **Run**



- Spacing of k-points: ***0.1*** 1/Ang
- select ***VASP settings***

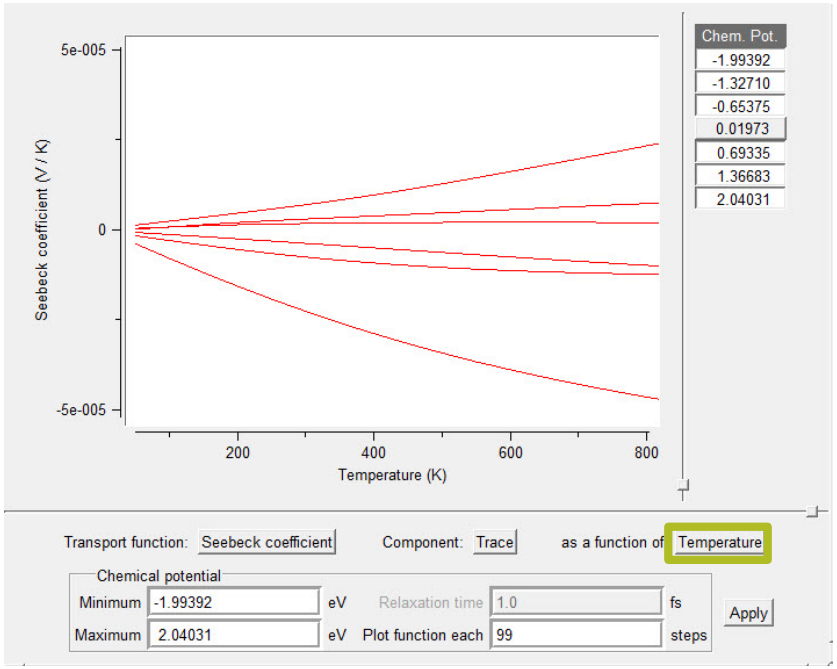
Submit MedeA® Electronics job

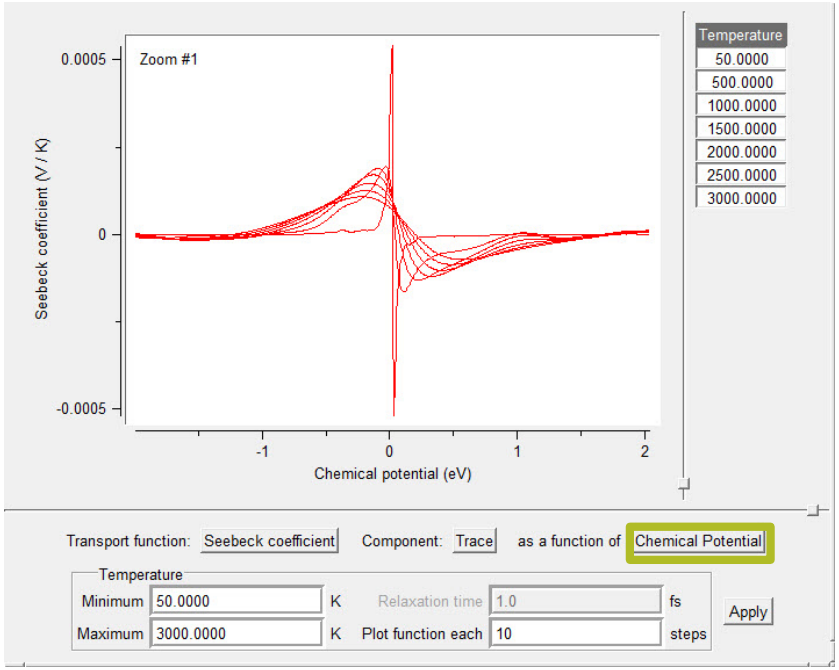
- In VASP GUI
  - ***Restore defaults***
  - Calculation type: ***Single Point*** **(Calculation panel)**
  - DFT exchange-correlation: ***GGA-PBEsol*** **(Calculation panel)**
  - Magnetism: ***Spin-orbit magnetic*** **(Calculation panel)**
  - Spacing of k-points: ***0.2*** 1/Ang **(SCF panel)**
  - ***OK***

- Back in Electronics GUI
  - Enter **Title:** *(Bi2 Te3)3 (R-3MH setting of R-3m) (Electronics)*
  - ***Run (Only set up the VASP jobs but do not actually run them!)***

- Check and analyse results:
  - ***Job Control*** → ***View and Control Jobs*** (opens JobServer interface in web browser)
  - Click on Jobs and afterwards on relevant job number of the running jobs
  - Check the progress of the calculation (indicated by **Available Results**)
- Display electronic transport properties
  - ***Electronics*** → ***Electronic Transport***
  - Select record of the relevant job
  - ***Insert >>***, ***Ok***

Analyze results for Bi_2Te_3

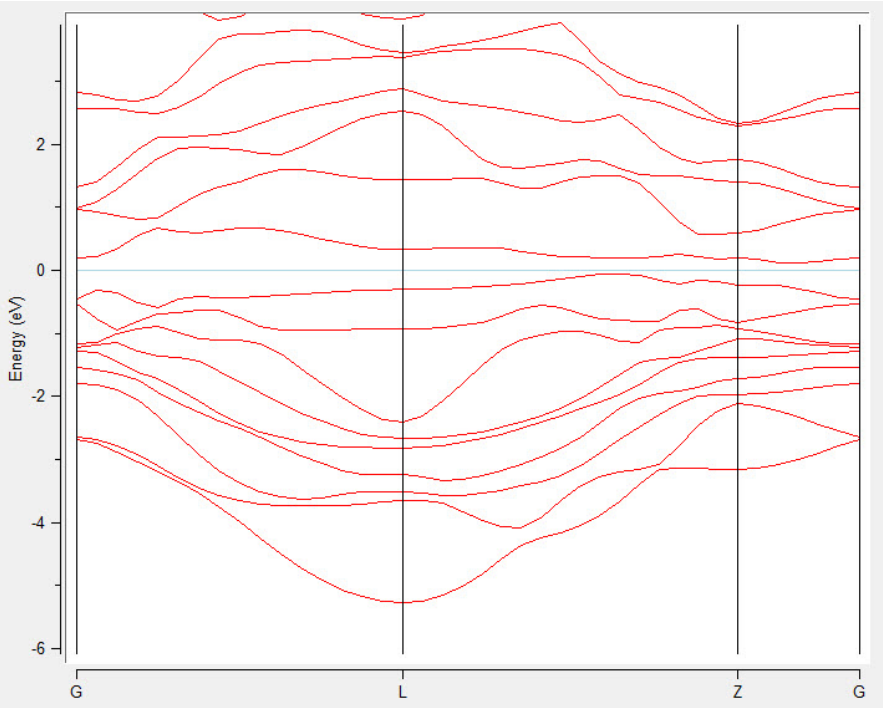


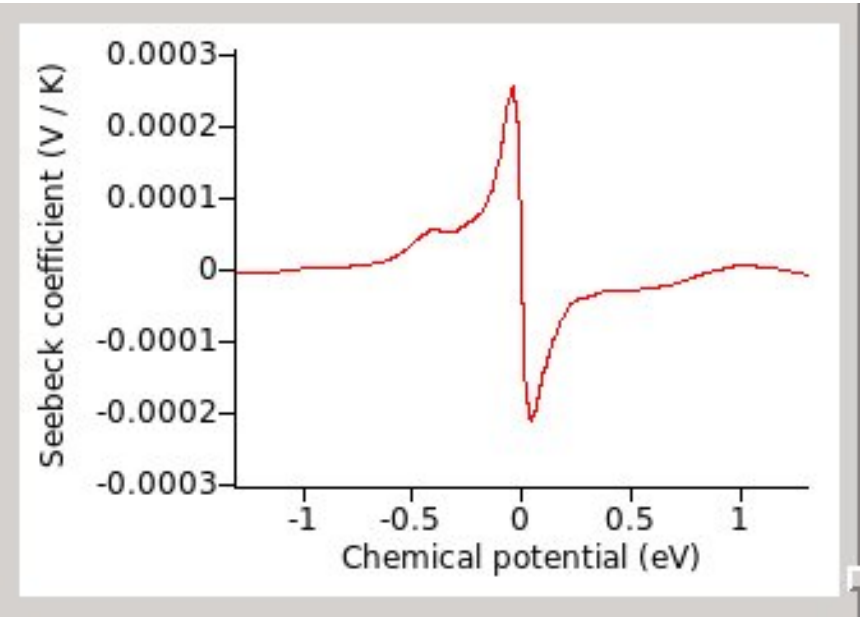


- display results as a function of
  - ***Temperature***
  - ***Chemical Potential***
- select/unselect single curves

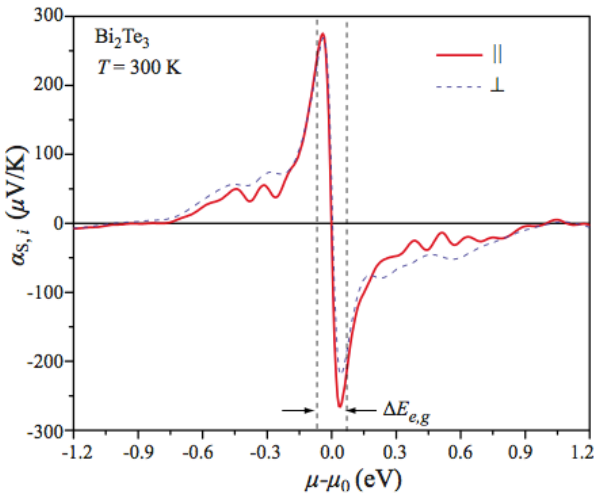
- thermoelectric power depends
  - strongly non-linear on doping
  - almost linear on temperature

MedeA® Electronics: Bi_2Te_3



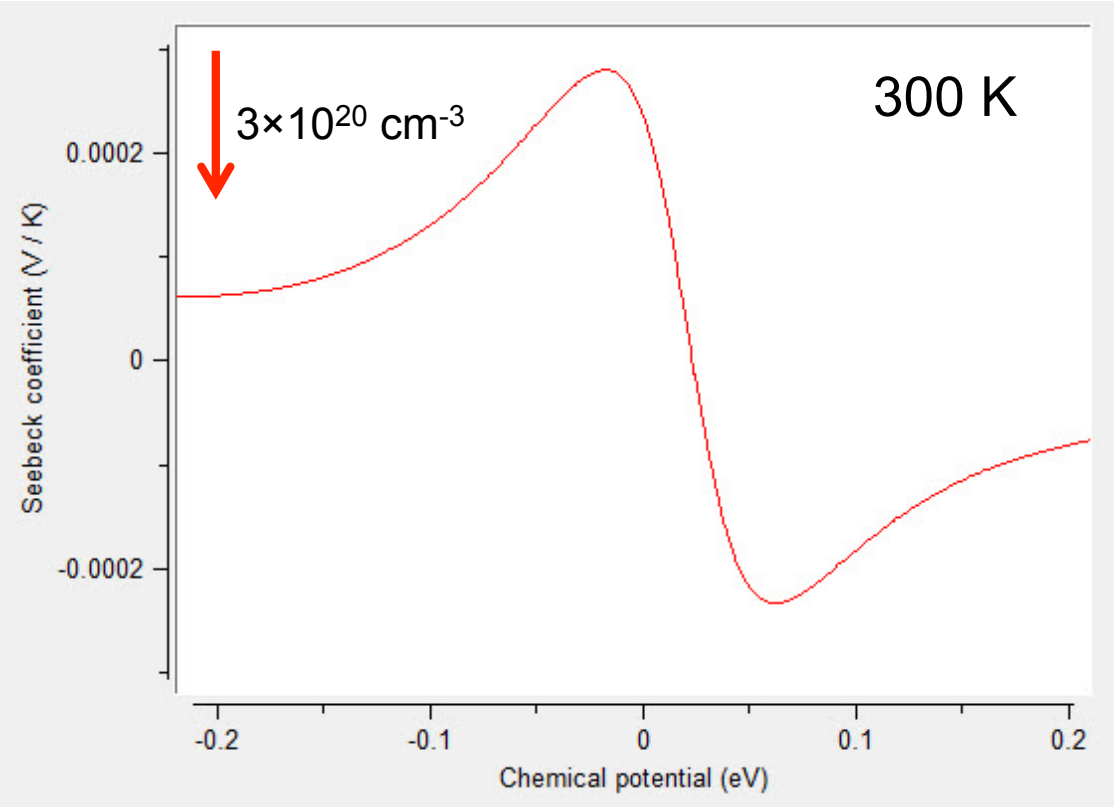


- indirect band gap, E_g=0.16eV
- experiment: E_g≈0.18eV
  (Sehr, Testardi, JPCS 1962)



Huang *et al.*, PRB **77**, 125209 (2008)

MedeA® Electronics: Bi_2Te_3

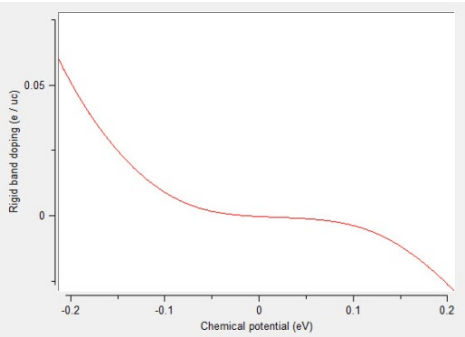


- experiments (RT)
  - S ≈ 260 μV/K at 4×10^{18} cm^{-3} p-type
  - S ≈ 250 μV/K at 7.4×10^{18} cm^{-3} n-type
  - S ≈ 287 μV/K n-type

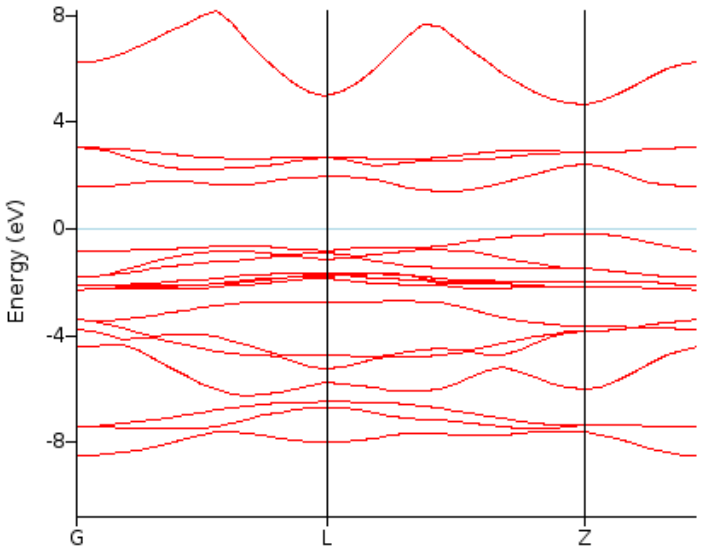
H.J.Goldsmid, Thermoelectric Refrigeration (NY, Plenum 1964)

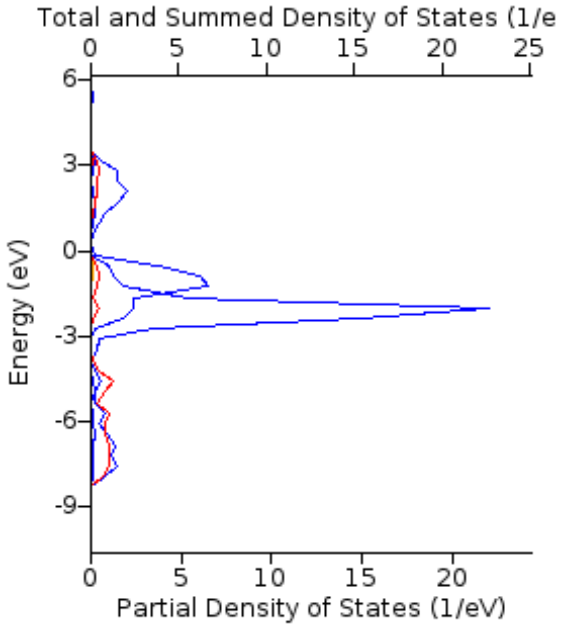
J. Tan, Proc. SPIE 5836 (2005)

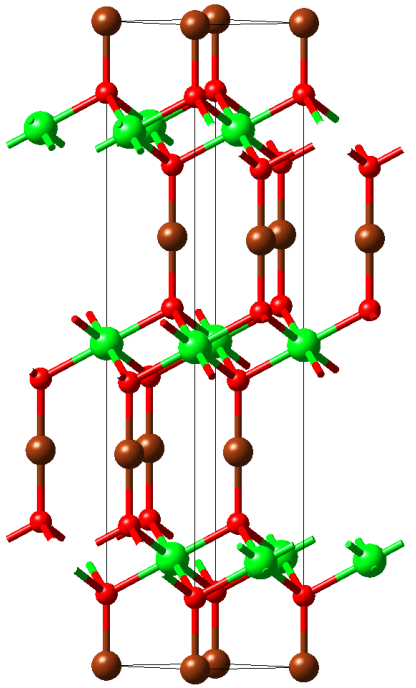
- calculated Seebeck coefficient
  - S ≈ 300 μV/K for p-type doping
  - S ≈ 220 μV/K for n-type doping



$CuRhO_2$: Thermopower





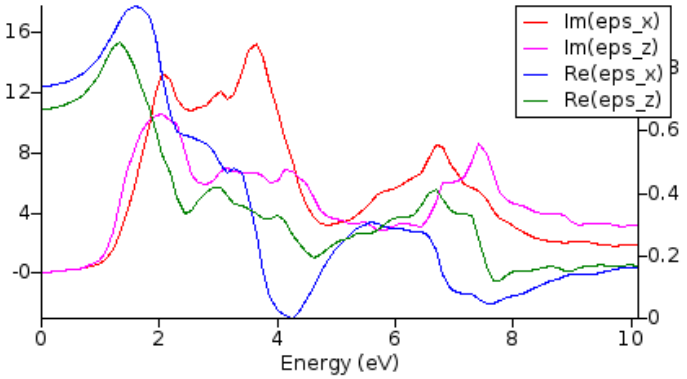


Cu

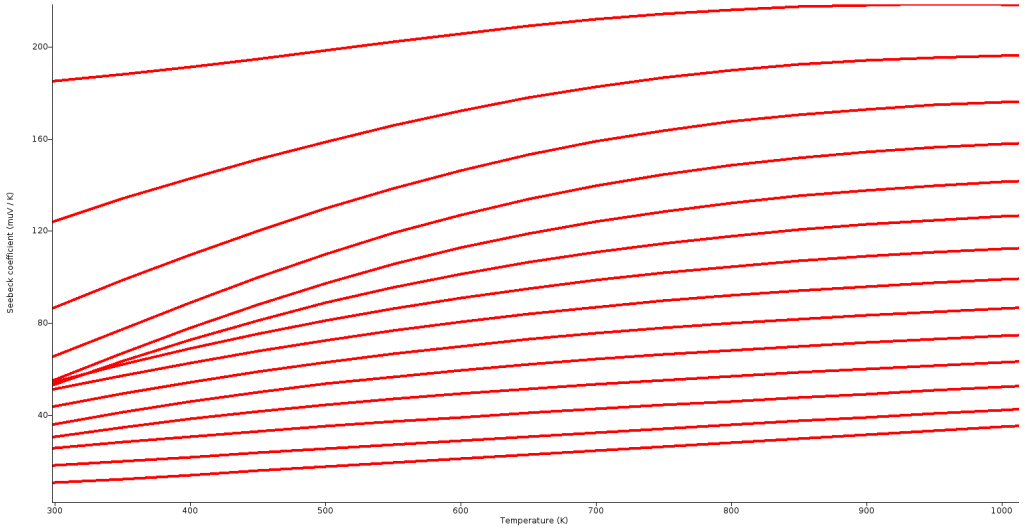
Rh

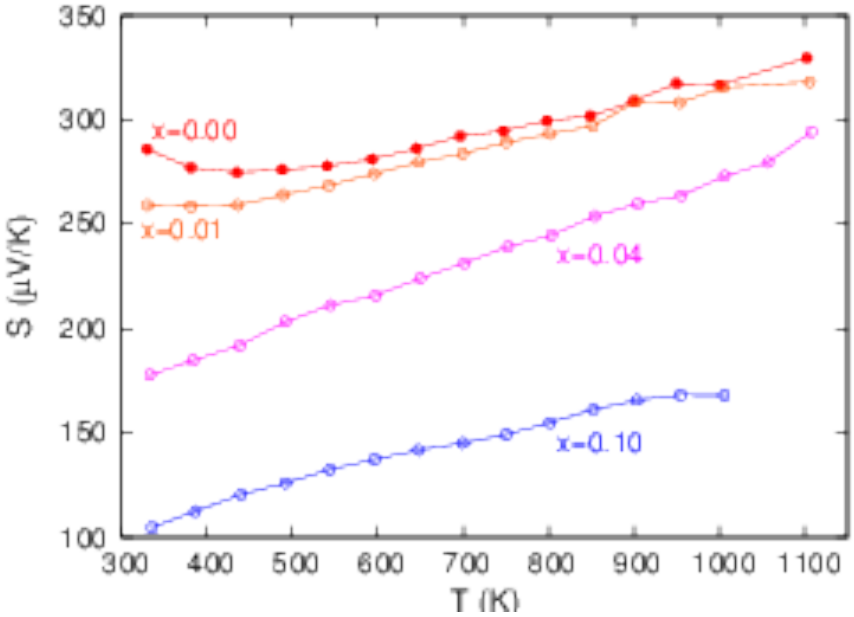
O

- delafossite structure
  - rhombohedral lattice
  - RhO_2 sandwiches (t_{2g}/e_g-splitting)
  - linear O-Cu-O bonds (sharp DOS-peaks)
- semiconductor
- $CuRh_{1-x}Mg_xO_2$: thermoelectricity



$CuRhO_2$: Thermopower





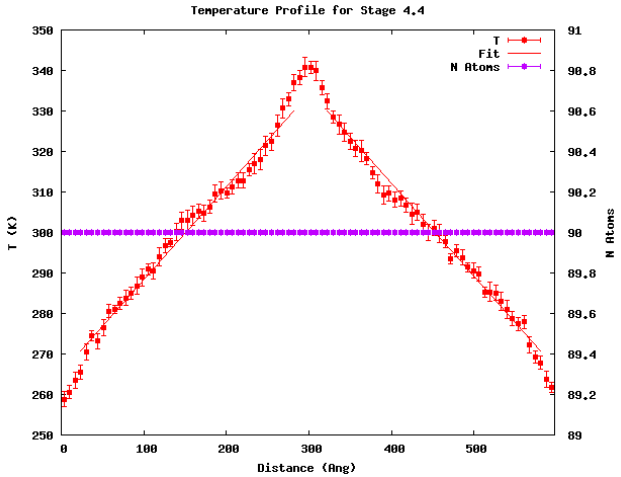
experimental data: A. Maignan, VE, C. Martin, S. Kremer, R. Frésard, D. Pelloquin, PRB **80**, 115103 (2009)

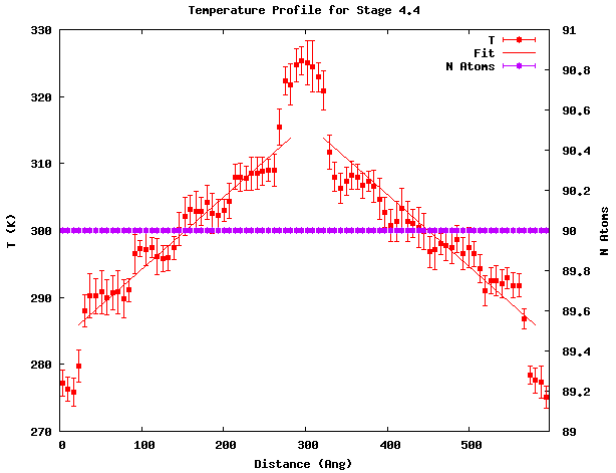
- good qualitative agreement
  - positive thermopower for hole doping ($0 < x < 10^{22}$ el/cm^3)
  - positive slope up to about 1000 K

Thermal Conductivity

Si-Ge Alloys: Thermal Conductivity

- Reducing the lattice thermal conductivity enhances *ZT*
- Improved understanding of the effect of composition and processing on thermal conductivity allows to tailor materials on the atomic scale



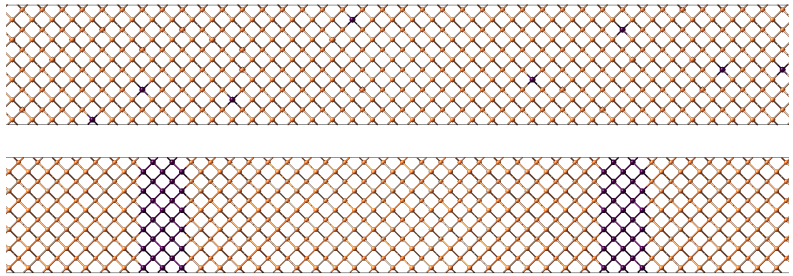


κ at 300 K in W/(m·K)

Sys.	Calc.	Expt(*)
Si	128	130
Ge	37	58

* Data from Ioffe Institute

System	Alloy	λ ($Wm^{-1}K^{-1}$)
$Si_{43}Ge$	random	6.87
$Si_{43}Ge$	layered	3.71
$Si_{43}Ge_5$	layered	1.87

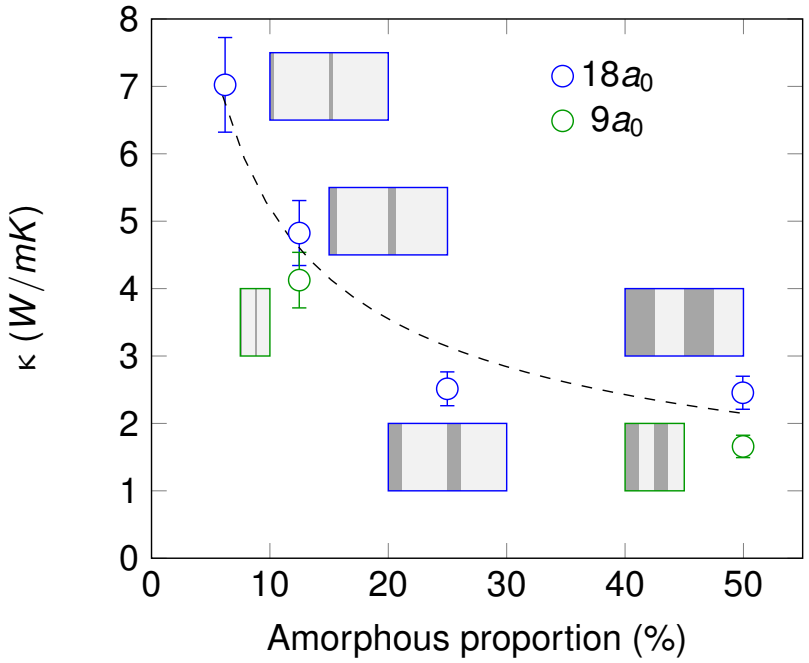


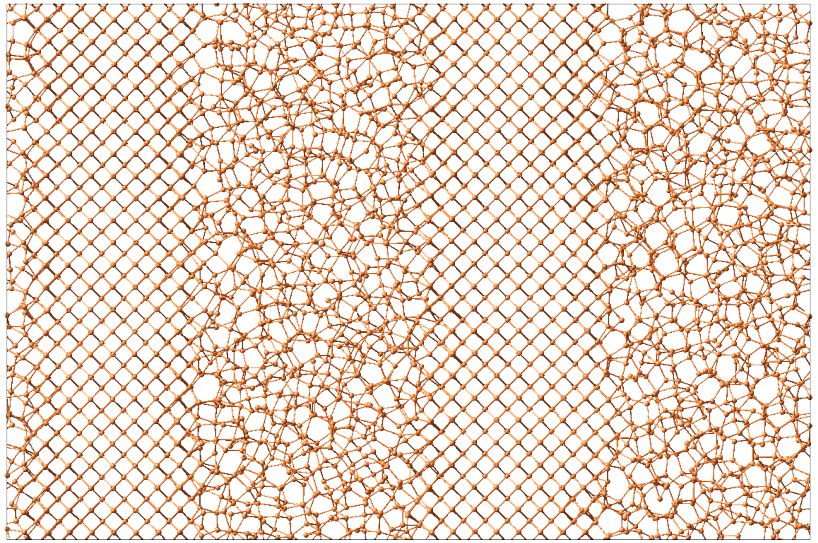
random Si_XGe_{1-X}

layered Si_XGe_{1-X}

a-Si/c-Si: Thermal Conductivity

- Introducing disorder can drastically reduce κ, and increase *ZT*
- This can be done without changing the composition of the system





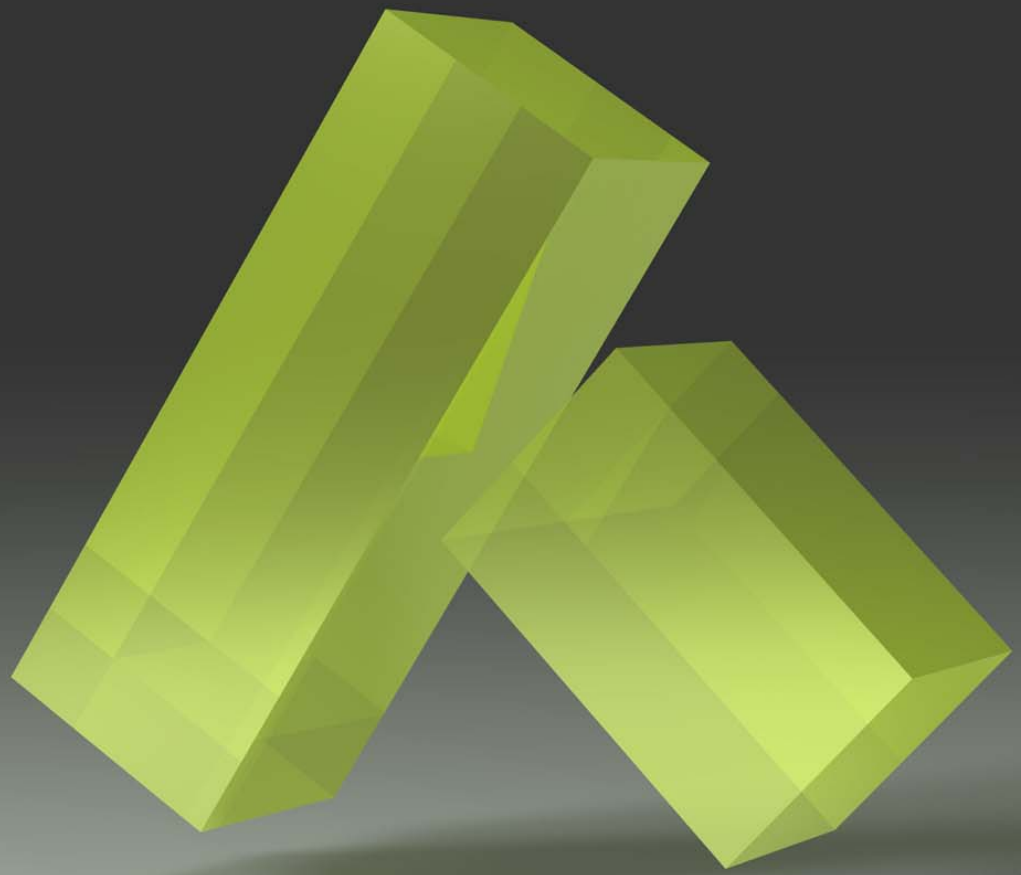
c-Si a-Si

- ~6% of amorphous Si is enough to reduce κ by a factor of 20!
- Thermal anisotropy, the ratio of $\kappa_{\text{in-plane}}$ and $\kappa_{\text{out-of-plane}}$: between 4 and 6

Summary and Perspectives

- DFT has become a standard in materials research
- A vast variety of properties can be routinely calculated
  - structural, mechanical, thermodynamic, kinetic, electronic, optical, magnetic, and transport properties
- Latest developments
  - Simulation of alloys: Universal Cluster Expansion
  - Automated forcefields from quantum mechanical calculations
  - Automation of simulation protocols (Flowcharts)

Better materials with better simulations



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MedeA® in Practice

MedeA® Software

MODELING & ANALYSIS

Builders: crystals, defects, interfaces, surfaces, molecules, nanostructures, polymers, amorphous materials

Analysis: geometry, band structures and DOS, electron and spin density, potential, Fermi surface, phonons, transition states, dynamics trajectories

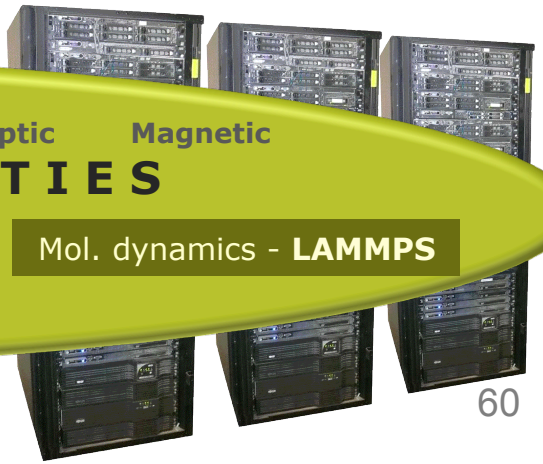
Job Server

DATABASES

Experimental and Computed Structure and Property Data

ICSD | NIST Crystal Data | Pauling | Pearson | Computed

Task Servers

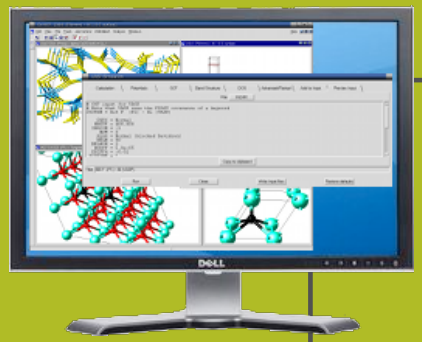


Mechanical Thermal Chemical Kinetic Electric Optic Magnetic

COMPUTATION OF PROPERTIES

ab initio QM - **VASP** | Semi-empirical - **MOPAC** | Monte Carlo - **GIBBS** | Mol. dynamics - **LAMMPS**

MedeA® Training Setup



User Interface

Model creation
and analysis of results

Local databases
(experimental and computed)

Local JobServer

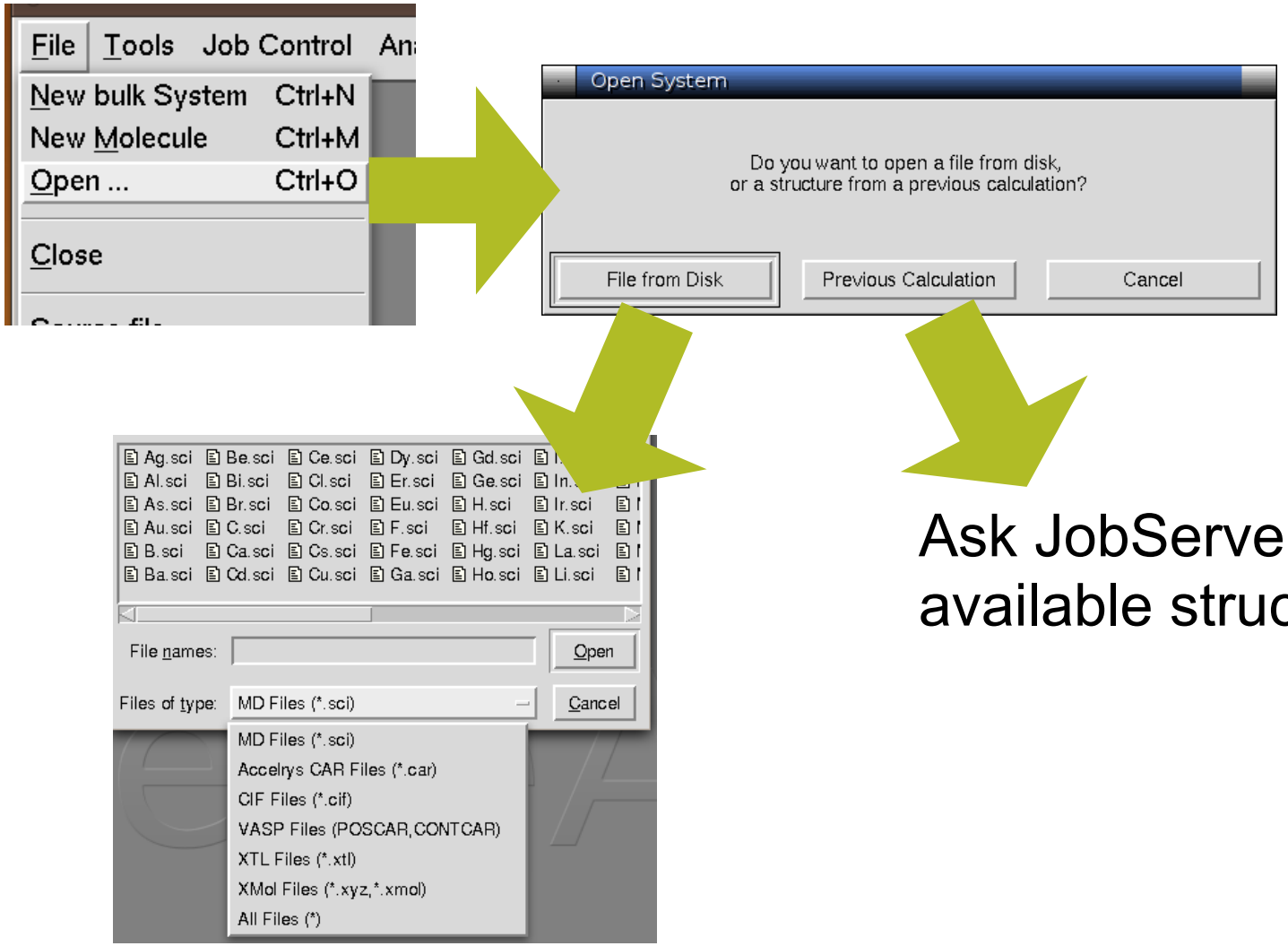
Loaded with completed
results of many
- Examples
- Structures
- Properties

Local TaskServer

multiple core processor computers
for serial and parallel calculations

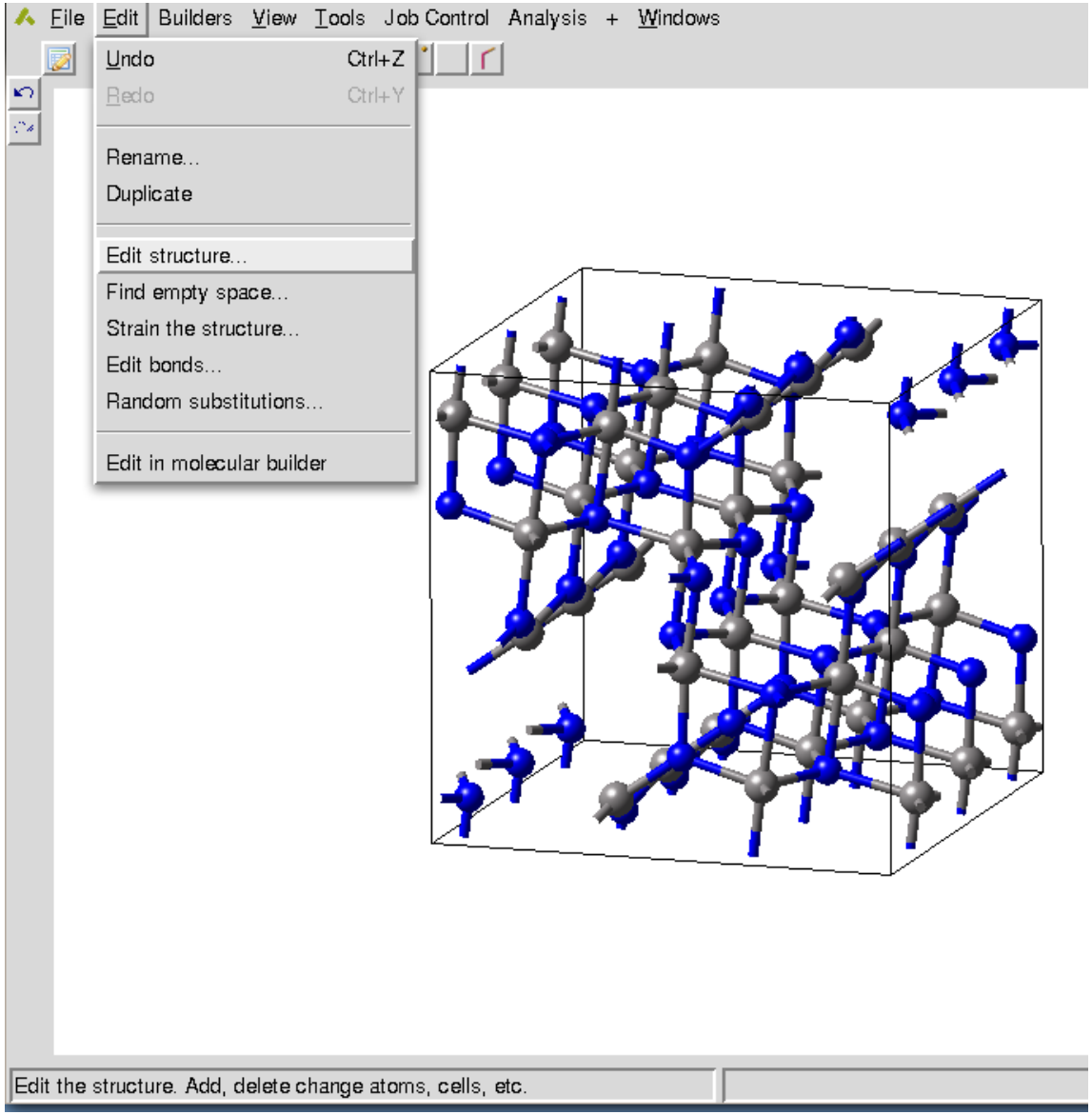
Access Structures

Load Structures



Ask JobServer for available structures

Crystal Structure Editor

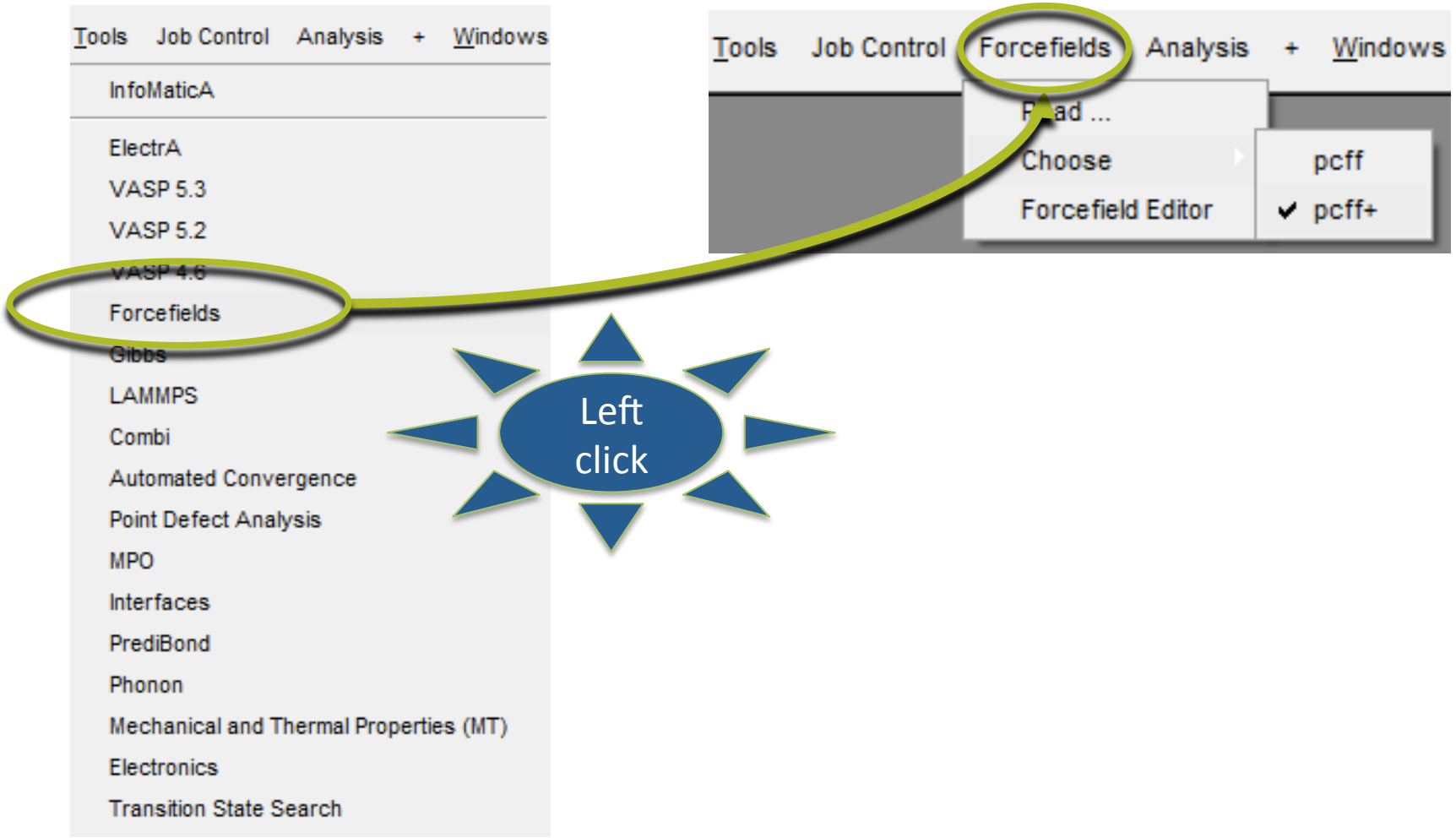


- Change lattice parameters
- Raise/lower symmetry
- Atom properties
  - Move
  - Edit (Replace)
  - Add
  - Freeze coordinates
  - Initial magnetic moment
  - Mass

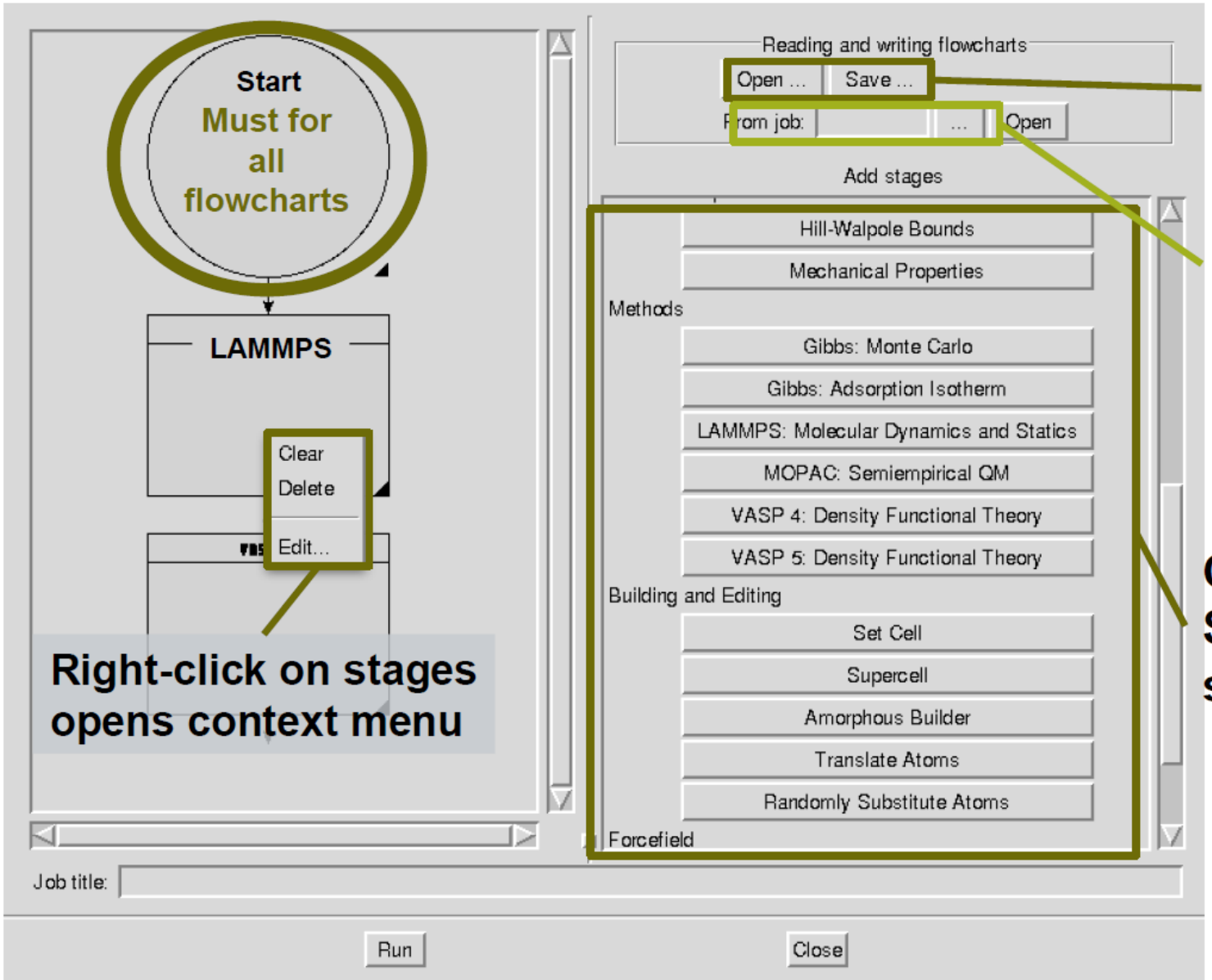
Keyboard Shortcuts

Ctrl **- Z**	undo the last action
Ctrl **- A**	select all atoms in the drawing area
Esc	clear the atom selection
Delete	delete all selected atoms
R/T/S/Z	press and hold down one of these keys to temporarily swap between the current mode and **R**otate/**T**ranslate/ **S**elect/**Z**oom
← → **+ R/T/Z**	**R** 1°/**T** 0.1 Å/small **Z**
Shift **+** ← → **+ R/T/Z**	**R** 10°/**T** 1 Å/big **Z**
← → **+ R/T + S**	**R**(→)/**T** selected atoms
↓ ↑ **+ R/T + S**	**R**(↑)/**T** selected atoms
Alt **+** one of the above	**R**-axis/**T** ⊥ image plane

Loading Tools to Menu Bar



Flowchart: Complexity Made Simple



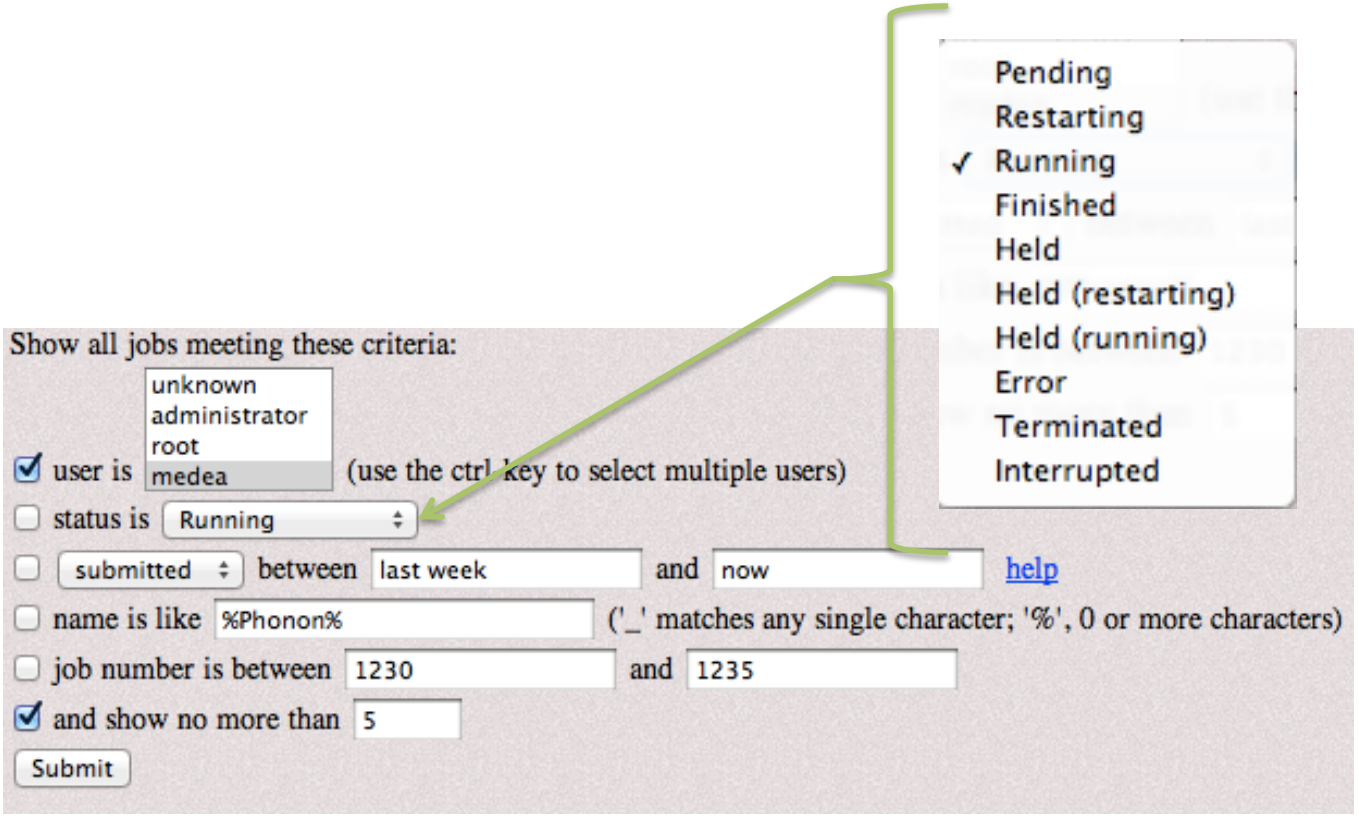
Read/save flowcharts from/to disk

Read flowcharts of previous jobs

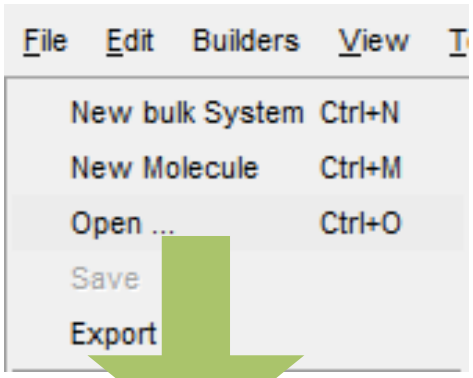
Click here to add Stages to the left side

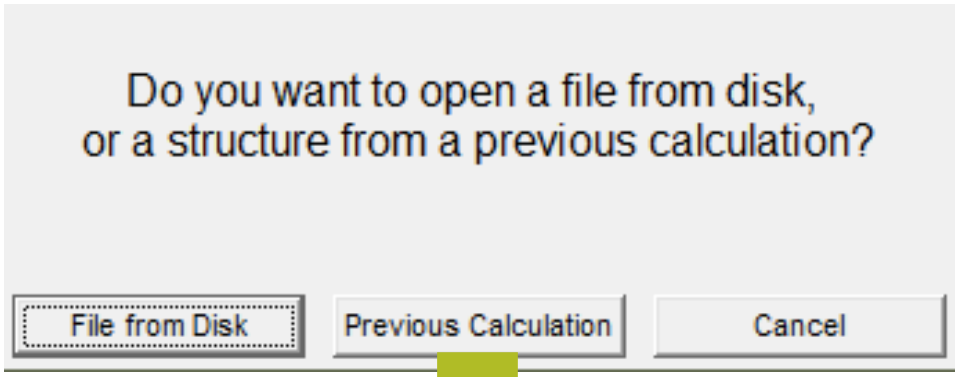
JobServer – Web Interface

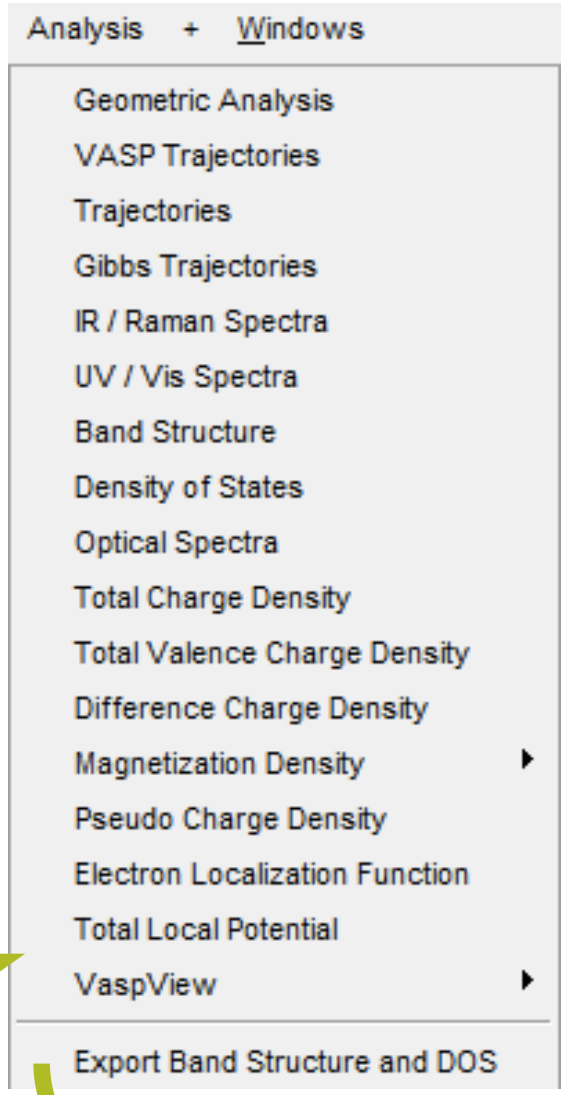
- Filter & Find
  - User
  - Status
  - Time
  - Number of Jobs to display
  - Start Over
    - Clean all results
    - Start from fresh Input files
  - Restart
    - Use existing files
    - Get files from completed tasks or redo missing tasks



Retrieve & Analyze Results





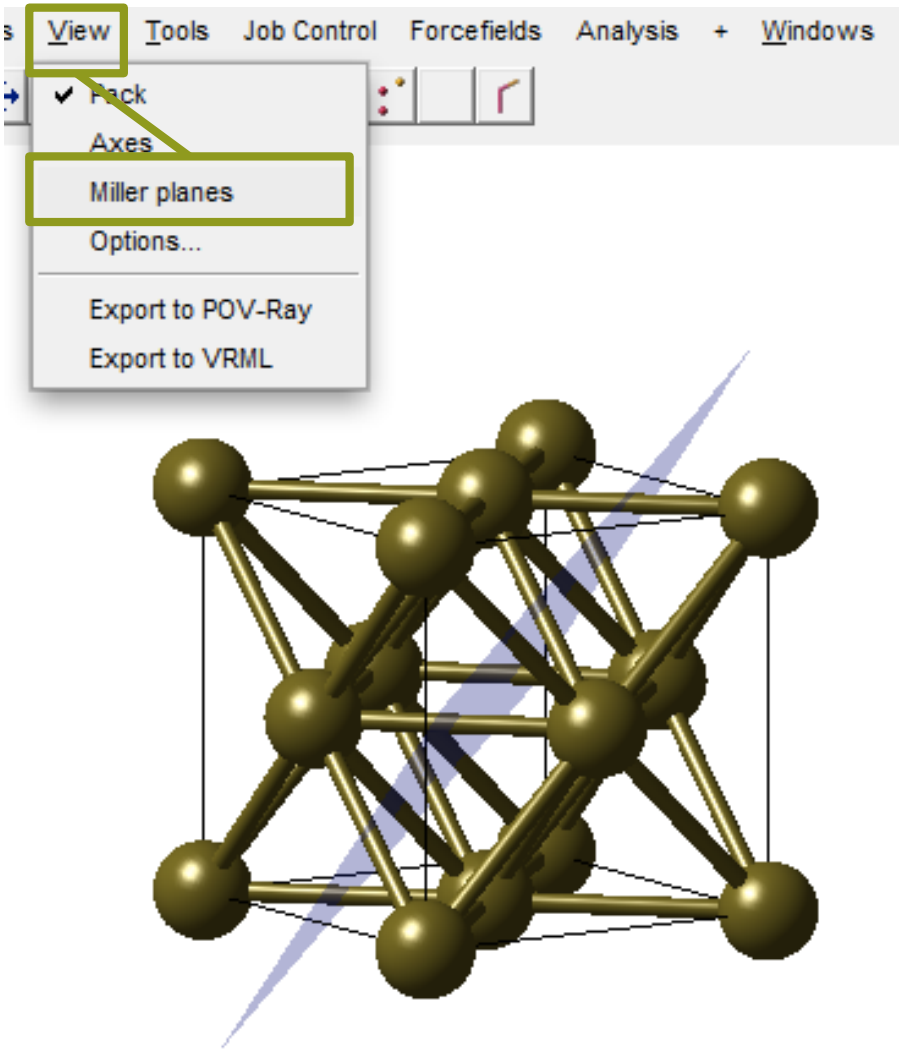


Contact JobServer for available results and data

Calls Microsoft Excel macro to create spreadsheet

Building Tools & Editors

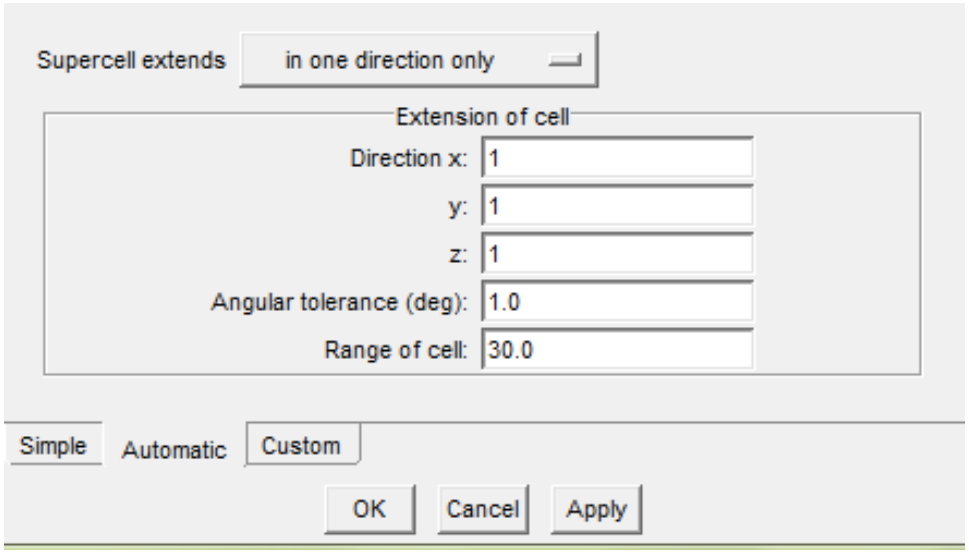
Crystal Planes



- File → Open → File from Disk
  - Browse to MD/Structures/Elements
  - Load Au.sci , Ag.sci, Pb.sci, …
- Display (1-11) Miller plane
  - Only for your guidance
  - No relevance in computation

Supercell Builder

- **Builders → Build Supercells…**
- Simple
  - NxMxO box
- Automatic
  - Equally in all directions
  - In one direction only
  - (h,k,l), range
  - … like surface builder



- Custom:
  - display hexagonal crystal in orthorhombic box
  - a'= {2 1 0 } a
  - b'=b
  - c'=c

Structures & Databases

MedeA® InfoMaticA

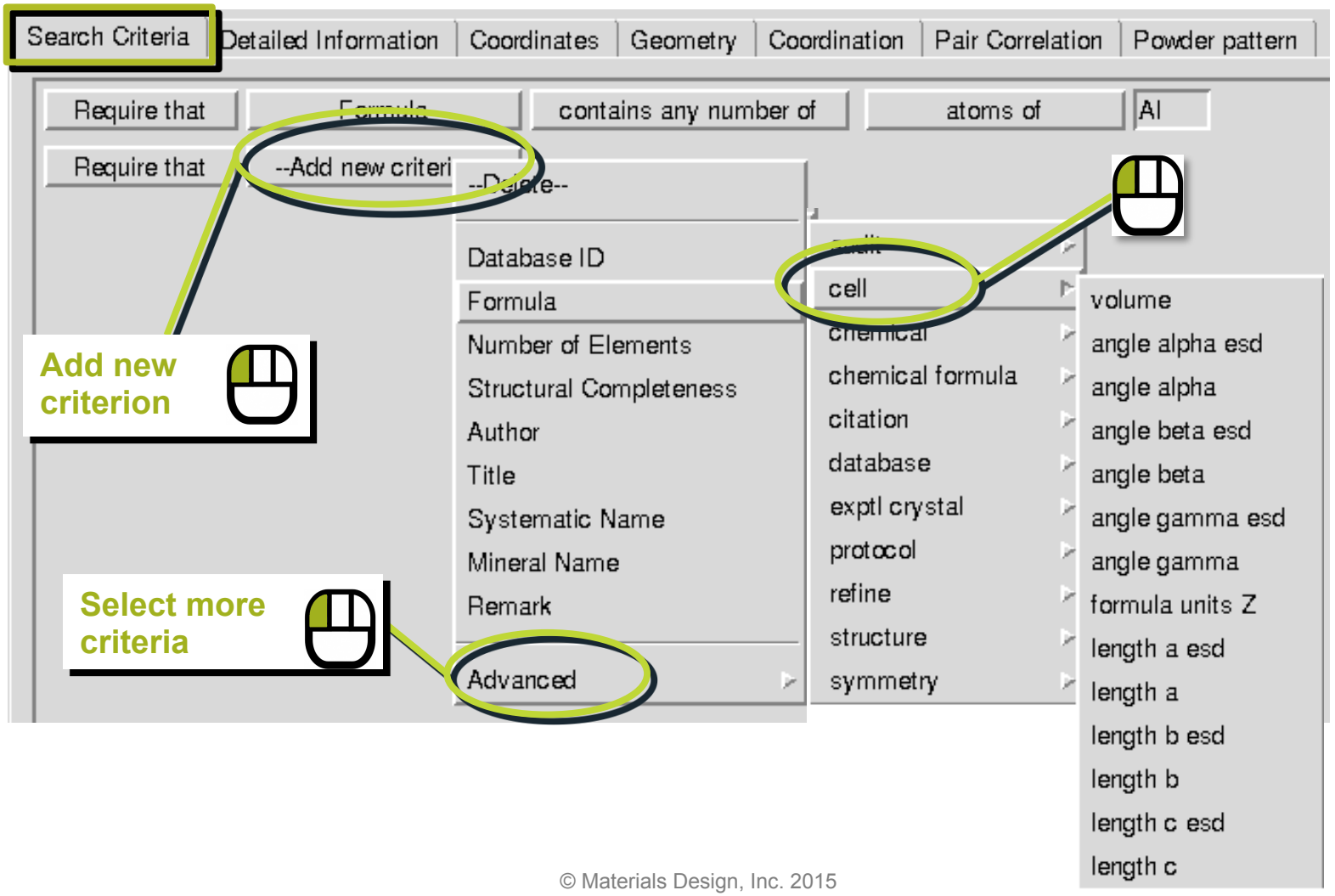
- Interface to the structure databases
  - ICSD ICSD (FIZ Karlsruhe, Germany)
  - Pauling (MPDS Projects, Switzerland)
  - Pearson (ASM International, USA)
  - NCD (NIST, USA)
  - COD (Cryst. Open Database)
- More thanthan **500'000** records in total
- Binary Phase Diagrams (Pauling)
- All records:lattice parameters (a, b, c, α, β, γ)
- Atomic coordinates depend on *structure type*
- Available *structure types*:

Type	Atomic coordinates	Site occupancy *n*
complete	all	1
disordered	over-complete	$0 \le n \le 1$
Missing atoms	incomplete	$0 \le n \le 1$
unknown	none	--

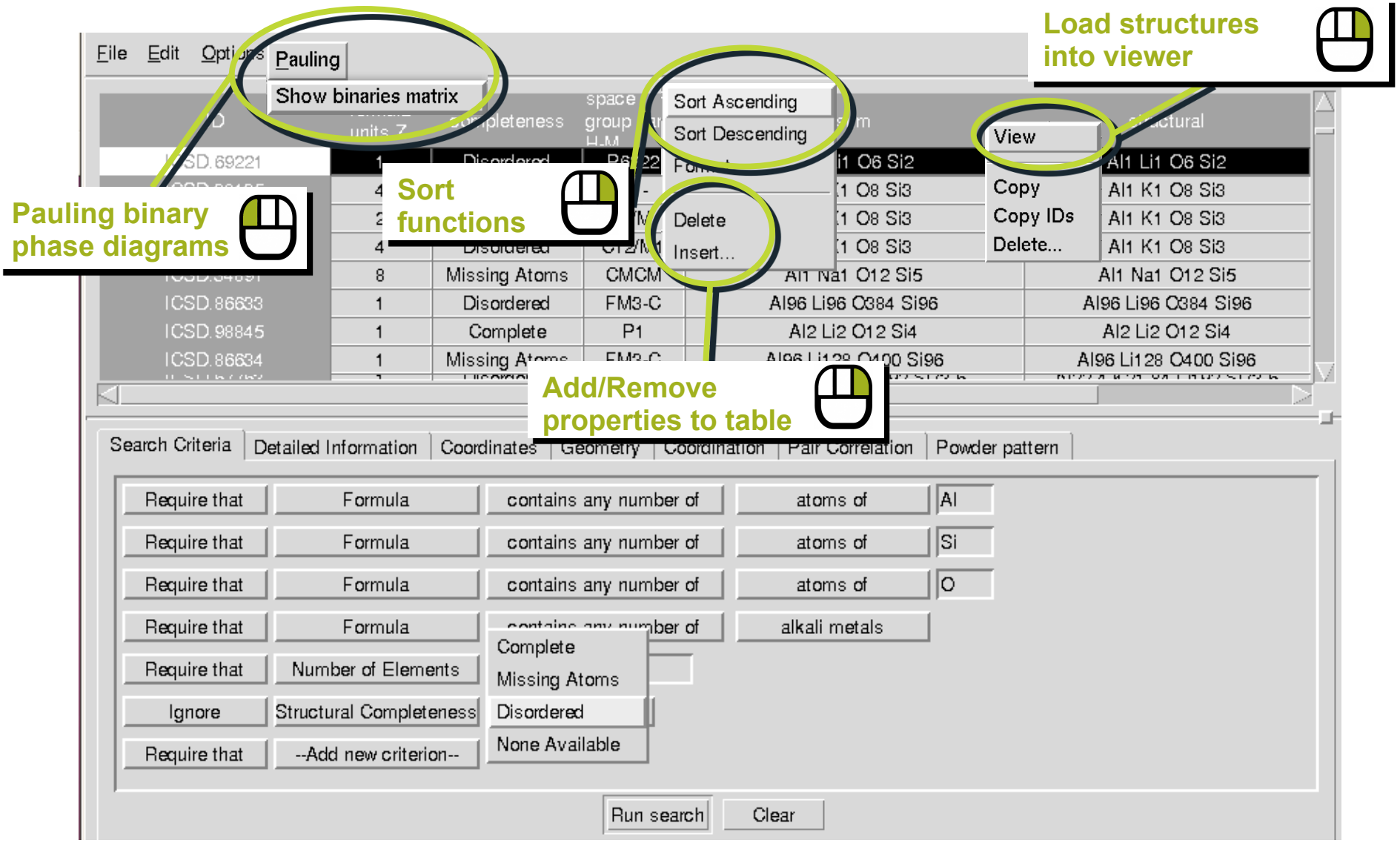
- Information on
  - Structures
  - Lattice parameters
  - Literature Data
    - Experimental setup
    - Phase information
  - Powder pattern
  - Coordination plots
  - Pair correlation function

InfoMaticA: Search Criteria

Open InfoMaticA: Tools → InfoMaticA, InfoMaticA → Search ..., panel **Search Criteria**



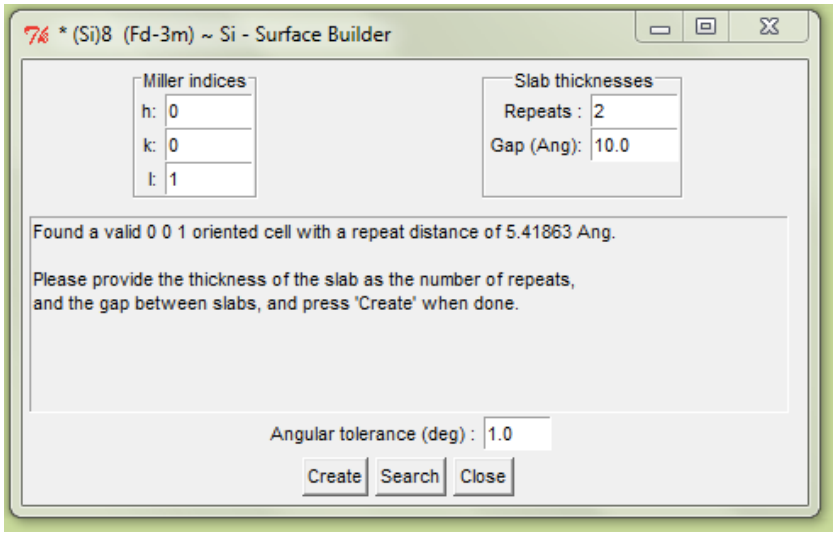
InfoMaticA: Search Mask

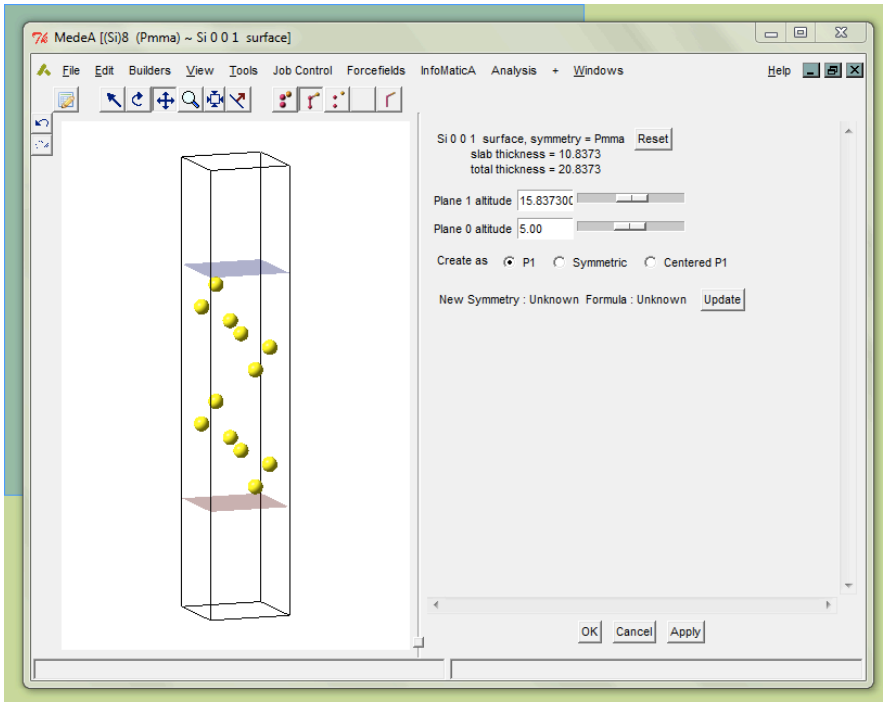


Surfaces

Si(001) Surface

- Define
  - Orientation
  - Repeat units
- Search
- OK

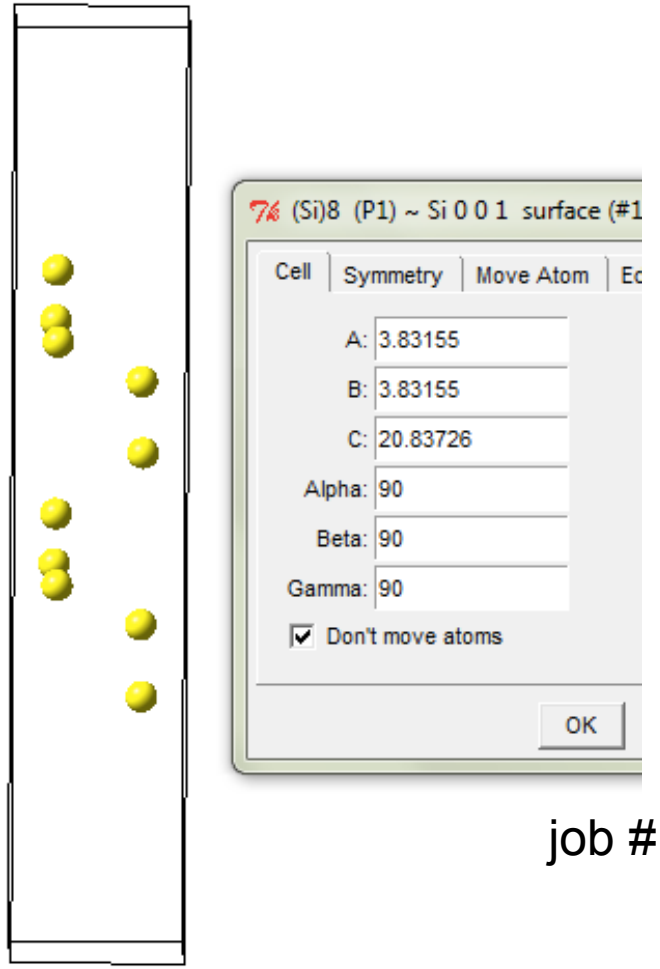




job #190

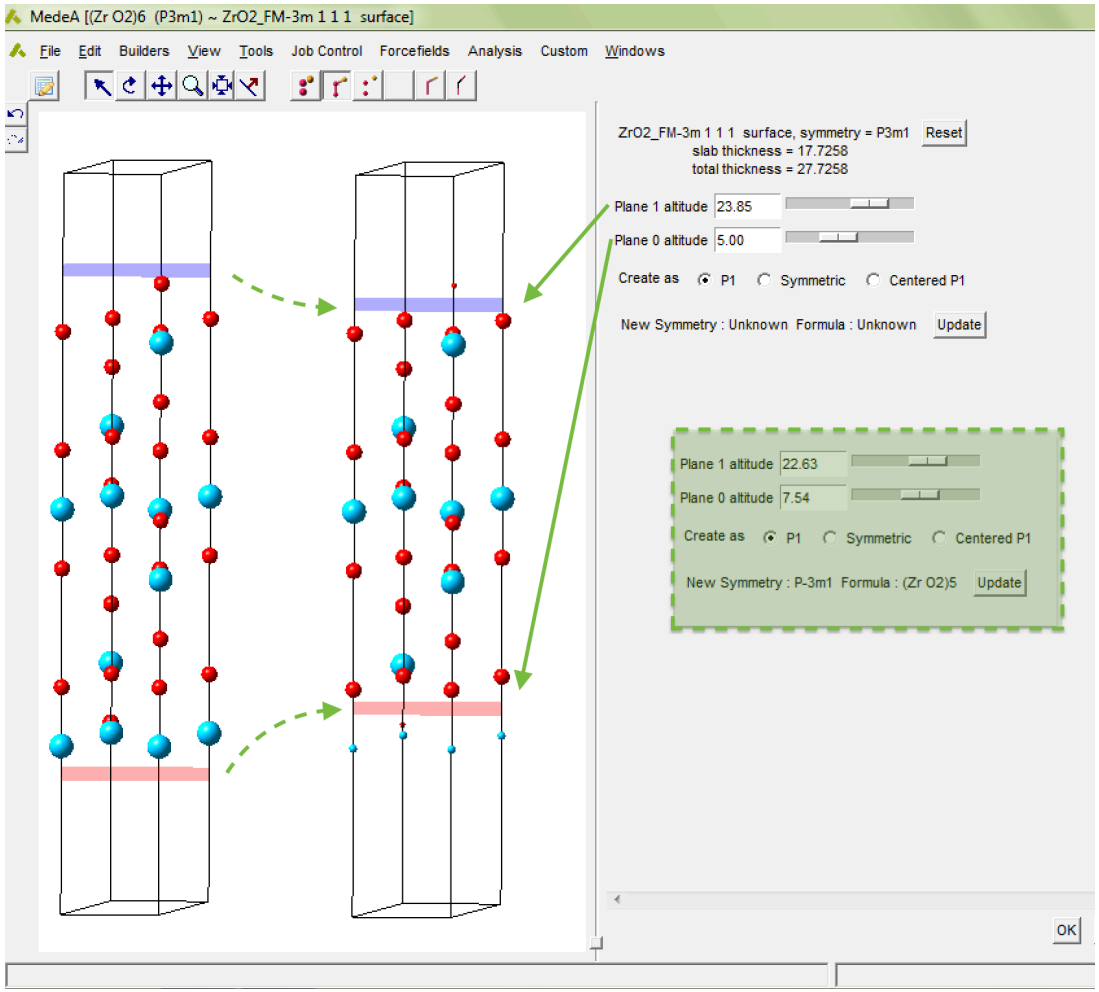
Si(001) Surface

- `Builders>>Build Supercell`
- 5x5x1 supercell
- Edit >> Cell
  - Menu or
  - Right-click
- Expand cell:
  - c=40 Å
- Don’t move atoms



job #190

Surface Termination



Move planes to exclude atoms

Tilt cell a little bit to see red and blue planes

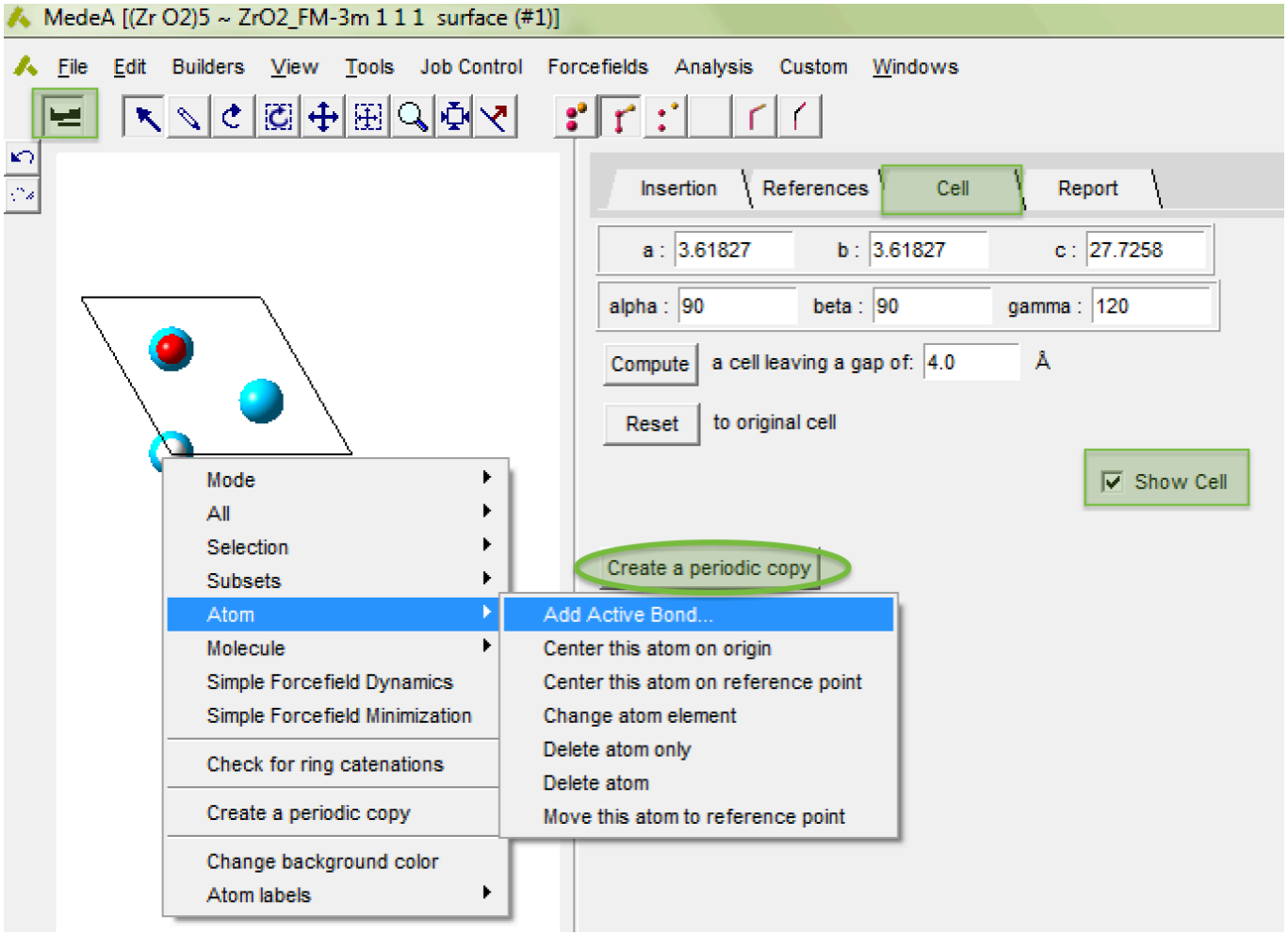
Update **symmetry** for Formula: (ZrO_2)

Impose symmetry?
Centered P1 moves slab into middle of cell (no effect on calculations)

Avoid polar surface slabs:
O termination on top,
Zr termination on bottom

Finish with **OK**

Preparing Surface Atoms



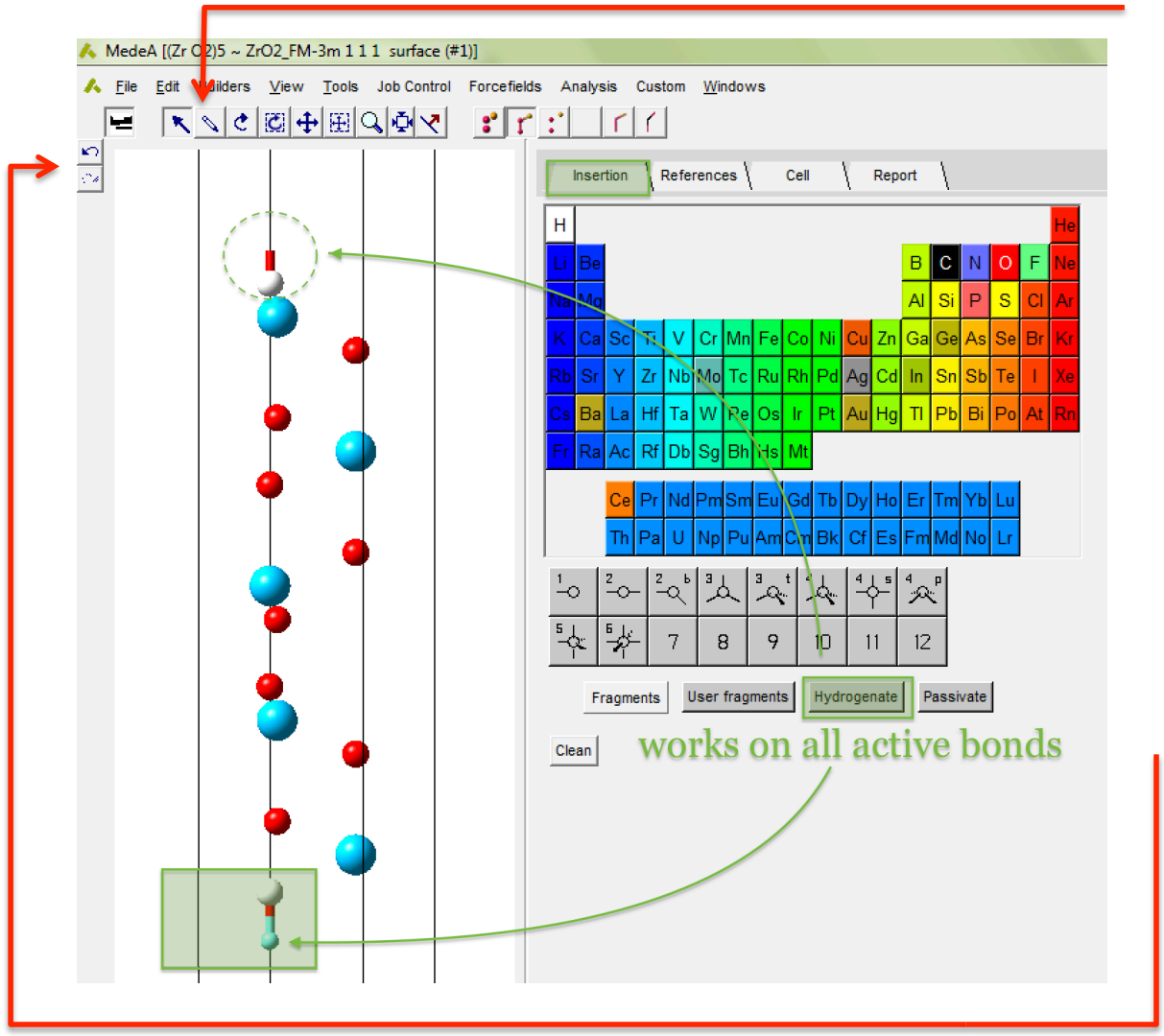
Click on **periodic table** icon

Model boundaries:
In Cell tab check
Show Cell

Select atom, right-click
Atom >> Add Active Bond…

Create a periodic copy when done

Surface Hydrogenation



Hydrogenate adds H to all active bonds

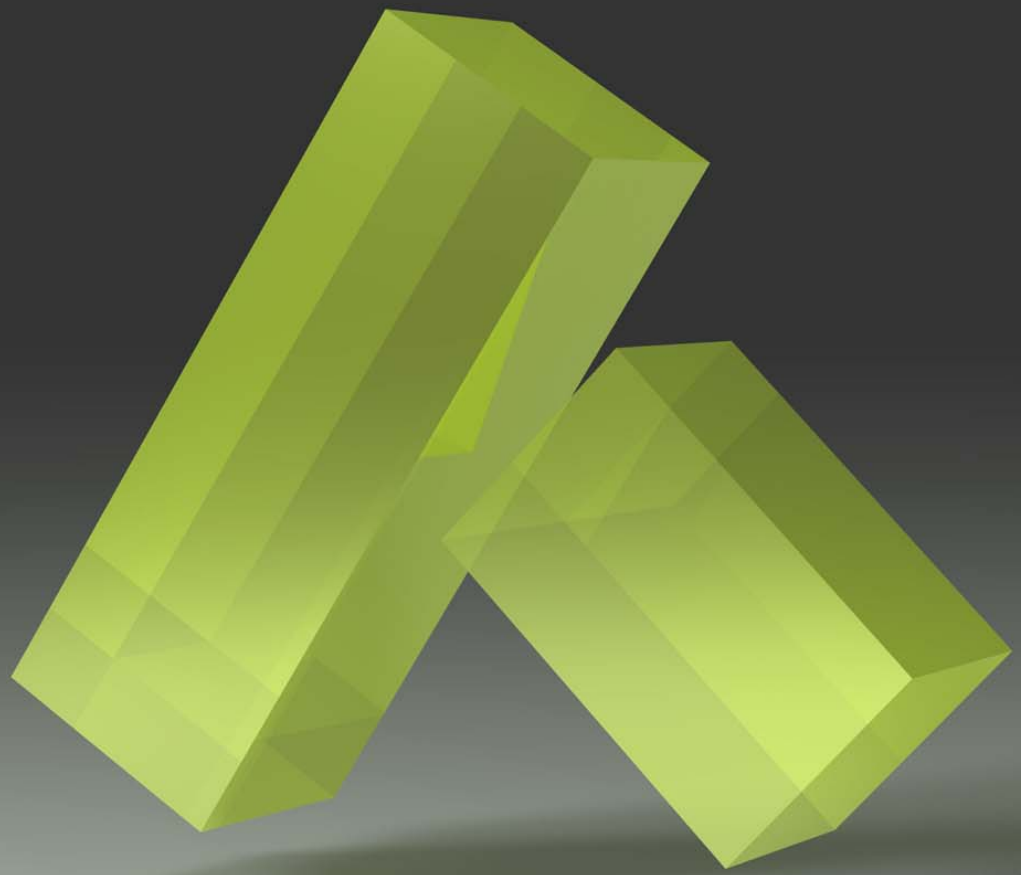
You can use any atom or group to **Passivate**

Use the sketch pen to draw molecules

Right-click: **Selection >> Simple Forcefield Minimization**

And don't forget: there is **Undo**

Better materials with better simulations



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