New ATK and VNL release 2017

highlights of new features and functionalities

Welcome! The webinar will start soon …

August 16 and 17, 2017
Live from Denmark and California

Webinar:
New ATK and VNL release 2017

Highlights of new features and functionalities

Presenters:
Umberto Martinez Pozzoni, PhD
Anders Blom, PhD

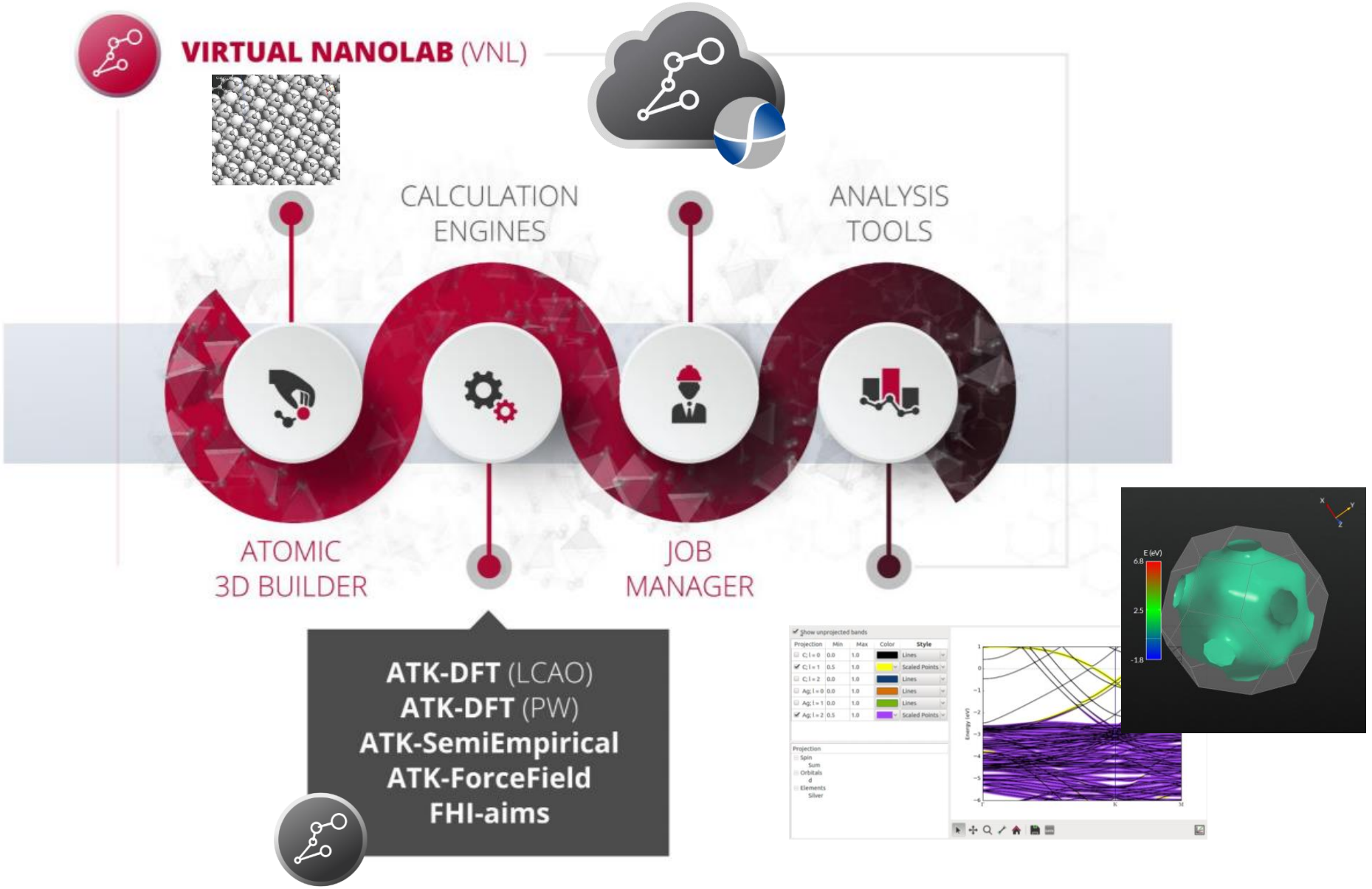
Quantum Wise

August 16 and 17, 2017
Live from Denmark and California

Agenda of today

1. QuantumWise
2. Important changes and highlights in VNL and ATK 2017
3. Performance improvements
4. New methods for band gaps
5. Wigner-Seitz approximation for large supercells
6. Demo: Fat band structures and projected density of states – Local job manager
7. Demo: Fermi surface analysis – Remote job manager/ATK on-demand
8. Demo: New functionality in the Builder
9. Demo: Connection to external databases
10. New features related to electron-phonon coupling calculations
11. Questions and answers

VNL/ATK platform workflow



Important platform changes in VNL and ATK 2017

- Only released on 64-bit platforms
- Mac OS X is discontinued
- ATK-Classical has been renamed ATK-ForceField
- Intel's mpiexec.hydra is provided on Windows and Linux
- New storage file format: HDF5
- Updated version of FHI-aims
- ABINIT removed from package

2017.1 bugfix update coming soon

See the official release letter for all details
http://quantumwise.com/about-us/quantumwise-news/item/1086-vnl-atk-2017-released

Highlights in VNL and ATK 2017 (not covered in this webinar)

- Quantum Espresso plugins updated to match latest QE version
- Surface configuration functionality mature
- Born effective charges
- Support for meta-dynamics using PLUMED
- ATK-PlaneWave (beta)
- …

See the official release letter for all details
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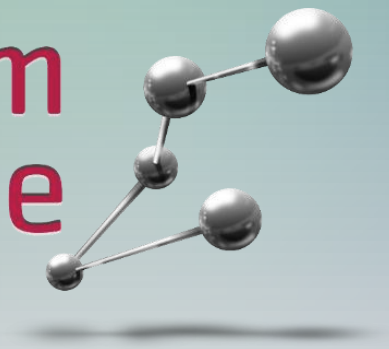
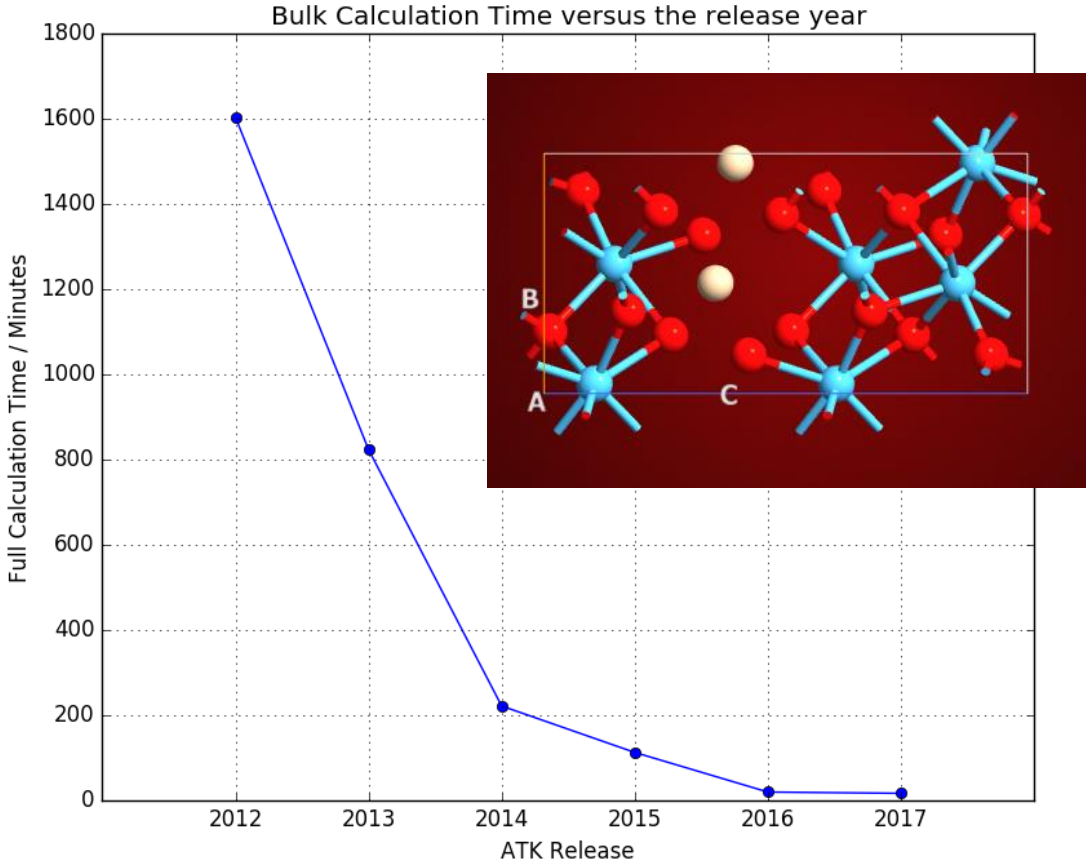
New in VNL-ATK 2017

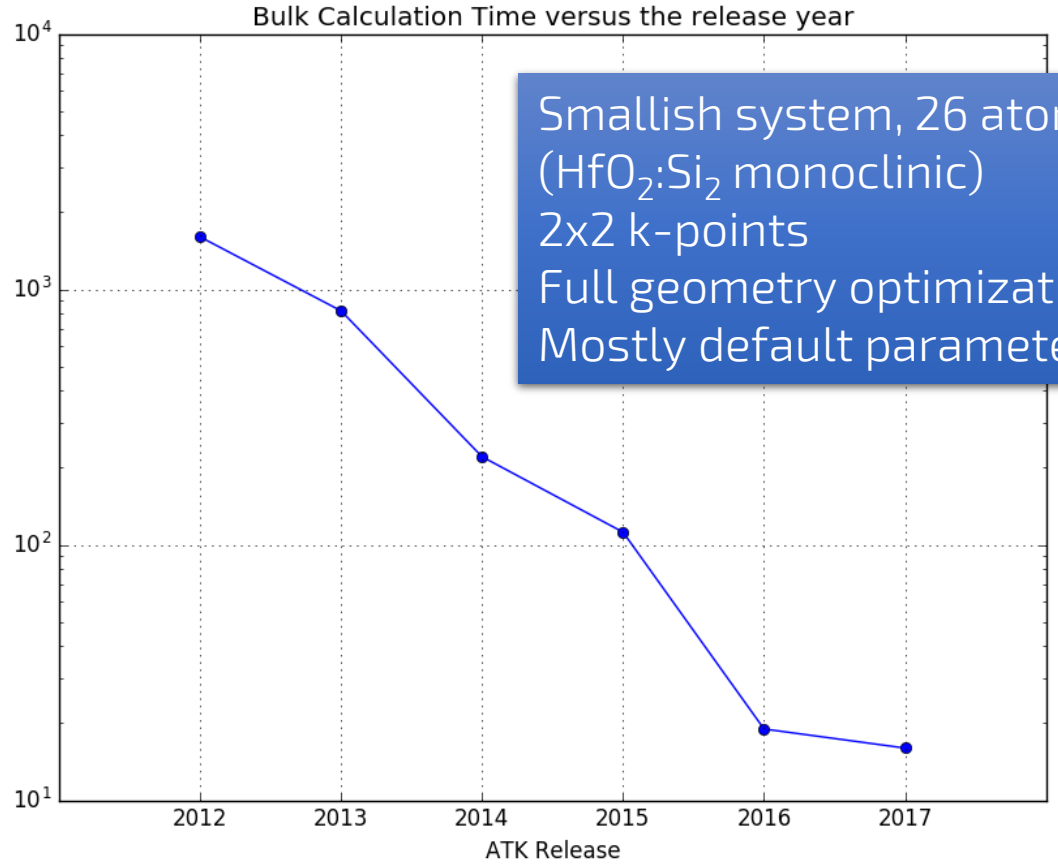
Anders Blom, CCO

Quantum Wise



Faster and faster…!





Smallish system, 26 atoms
(HfO_2:Si_2 monoclinic)
2x2 k-points
Full geometry optimization
Mostly default parameters

Performance improvements and new defaults

- "Bands above Fermi level" is now set automatically
  - Can give 2x performance, esp. for large systems
  - Could be set manually in ATK 2016 (but most users did not)
- SG15 Medium is now default basis set (slower, but more accurate)
- Basis-set specific default mesh cut-off
- GGA new default (was LDA)
- Electron temperature 1000 K
- NeutralAtoms is default (was EquivalentBulk)

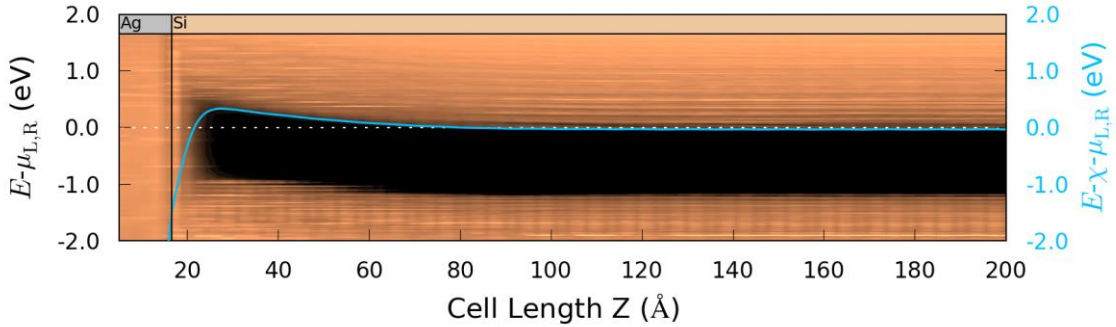
NOTE

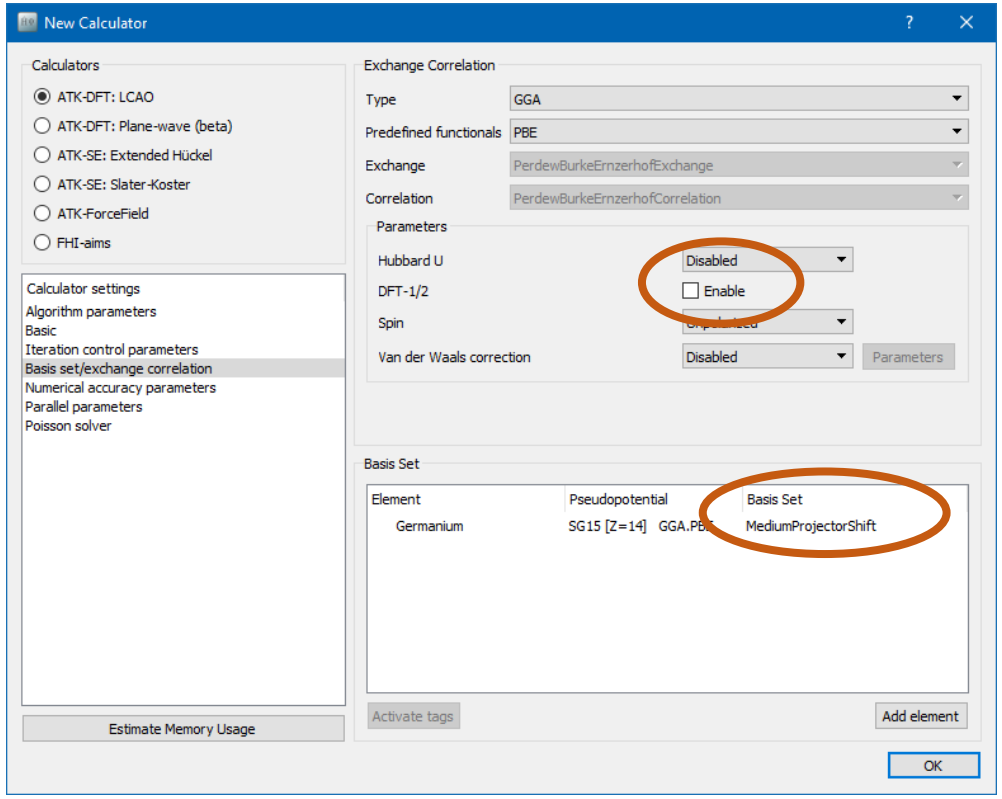
As a result, calculations run with minimal scripts, or by making a new script in VNL 2017, may differ from corresponding results in 2016 and earlier versions

Band gaps

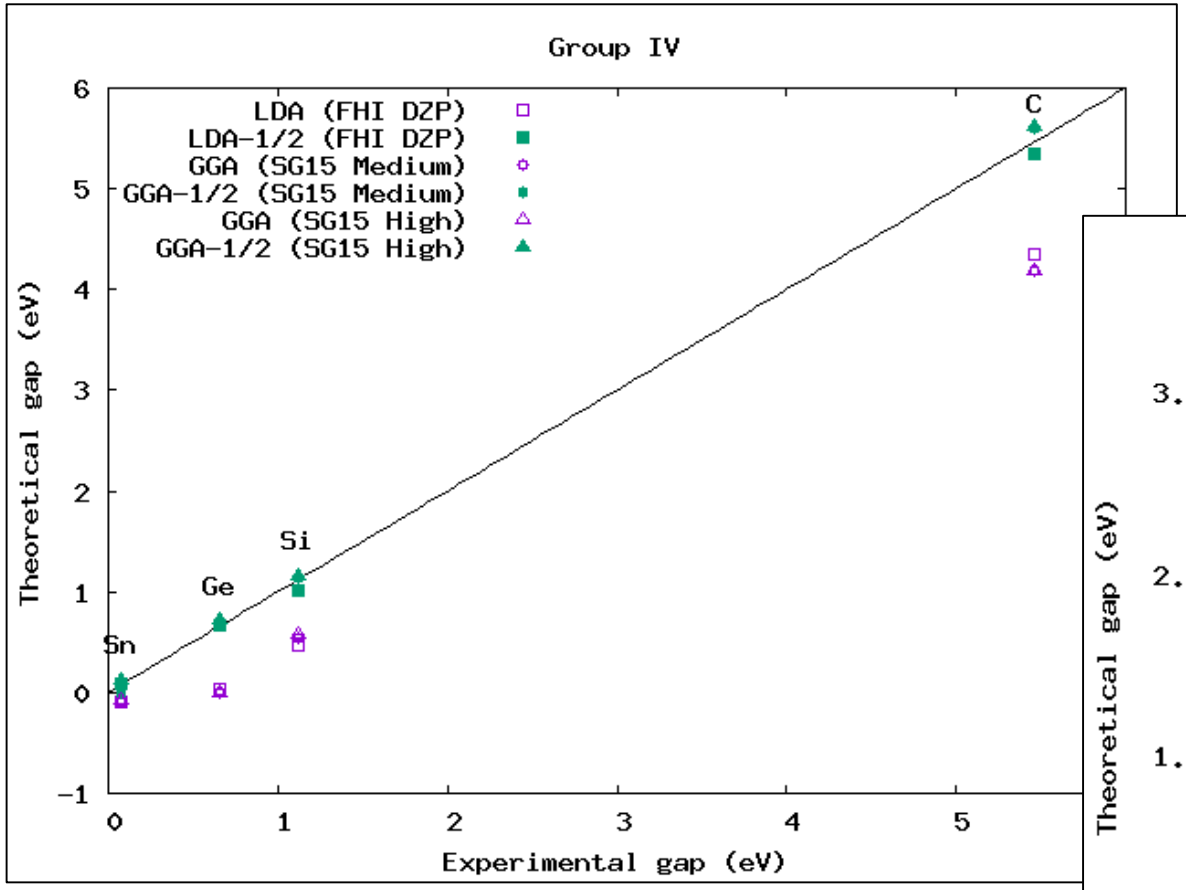
- Earlier methods in ATK for band gap corrections:
  - DTF+U
  - MetaGGA (TB09)
- Two new methods for (accurately) calculating band gaps are included in ATK 2017:
  - DFT+1/2
  - Pseudopotential Projector Shift (PPS)

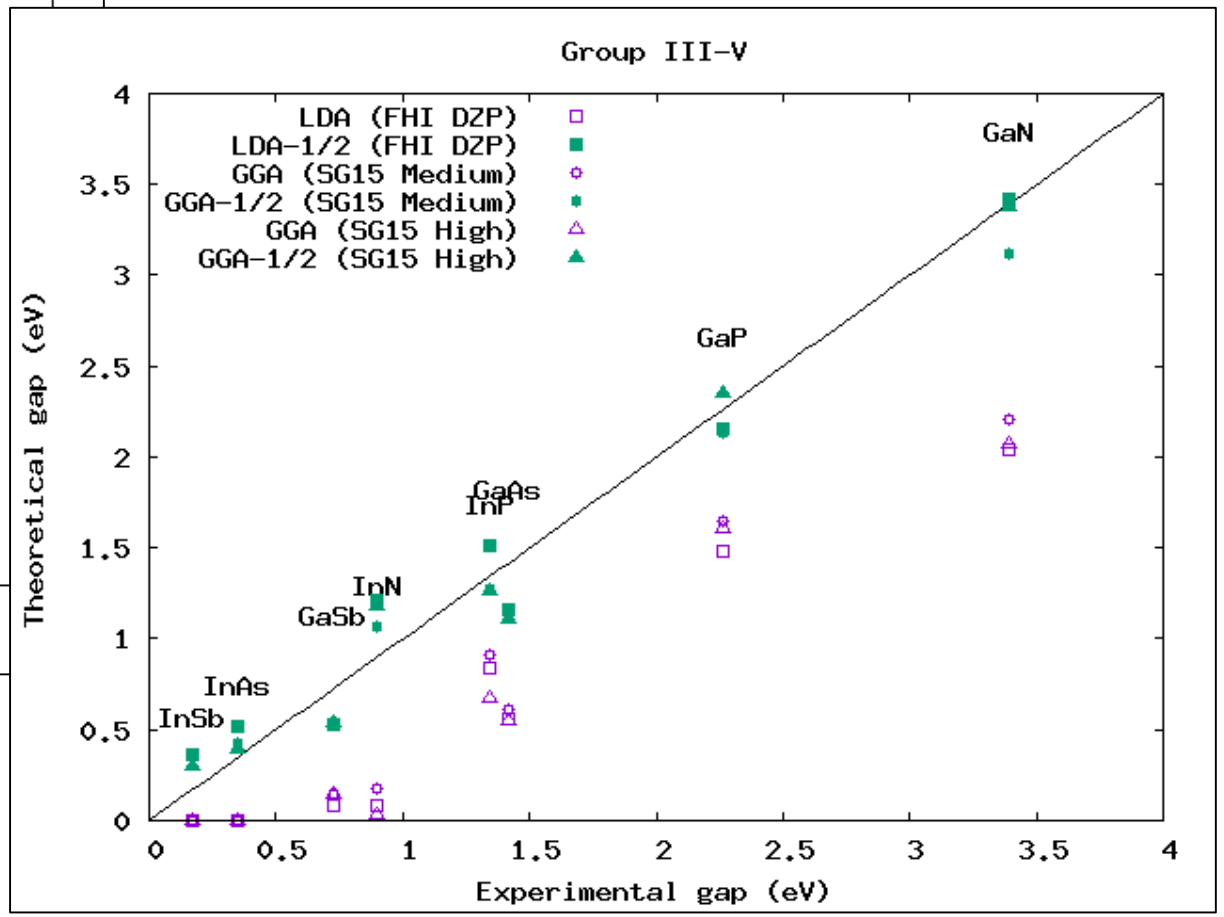
http://docs.quantumwise.com/tutorials/dft_half_pps



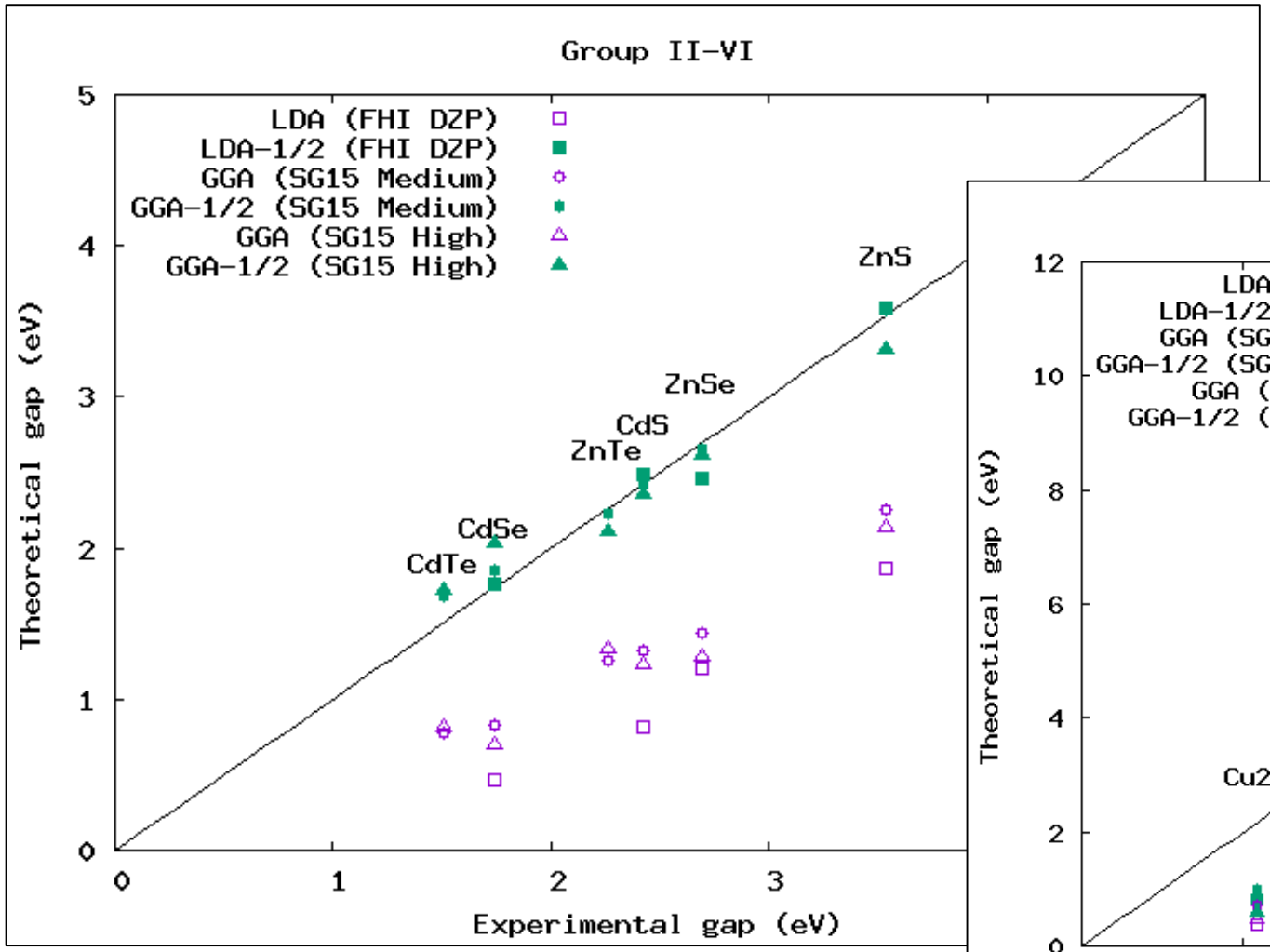


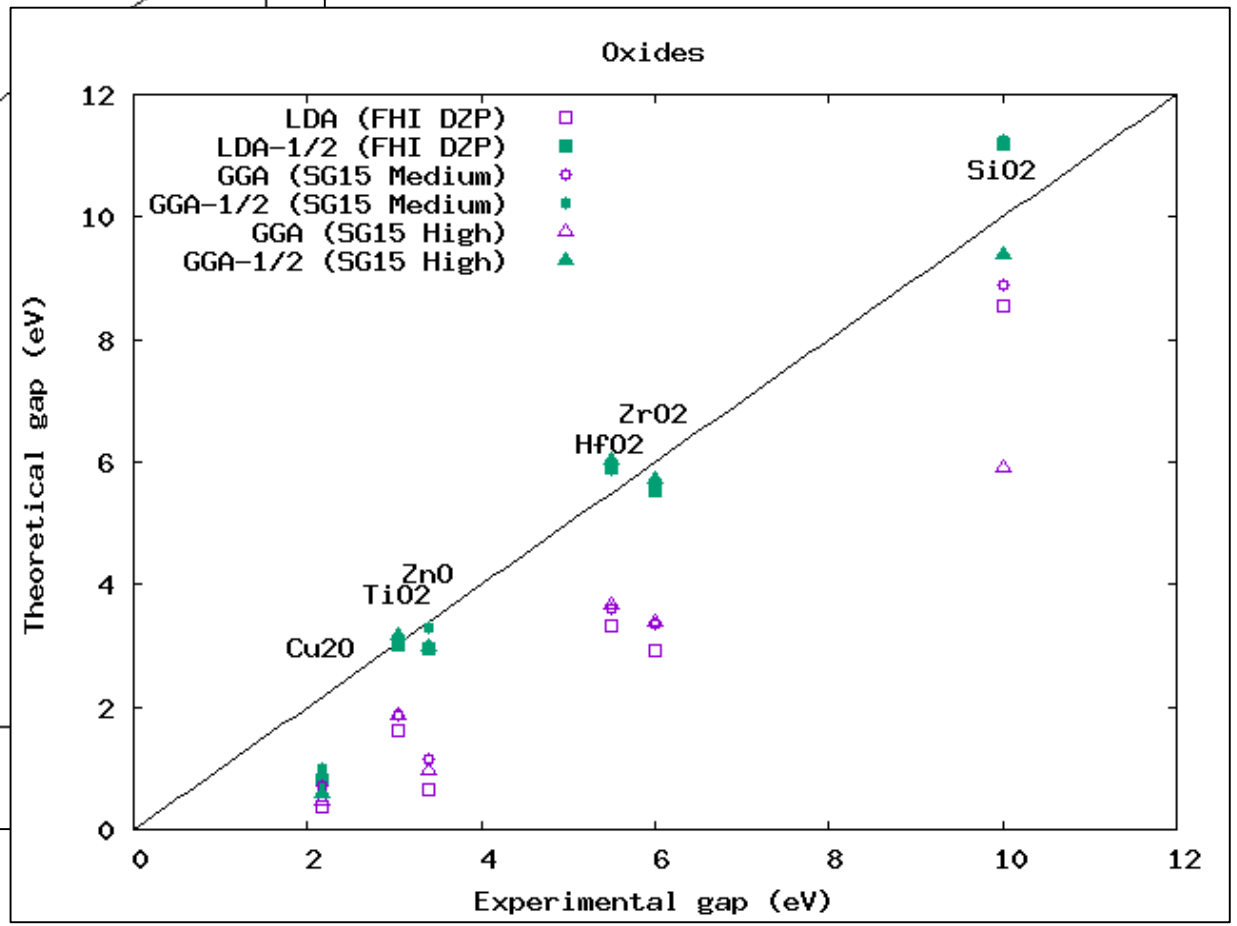
DFT+1/2: III-V and group IV





DFT+1/2: Oxides and II-VI





DFT+1/2

- Semi-empirical approach to correct the self-interaction error in local and semi-local exchange-correlation functionals
- Known from literature (Ferreira) and builds on Slater's half-occupation method
  - L. G. Ferreira, M. Marques, and L. K. Teles, Phys. Rev. B **78**, 125116 (2008), AIP Adv. **1**, 032119 (2011)
- "More ab initio" than other methods like MGGA or GGA+U
- Typically only need to provide parameter for the anion (like oxygen) which then works for all cations of the same oxidation state
- Not recommended for force/stress optimization
- Parameters provided for common semiconductors
  - Possible to fit your own parameters

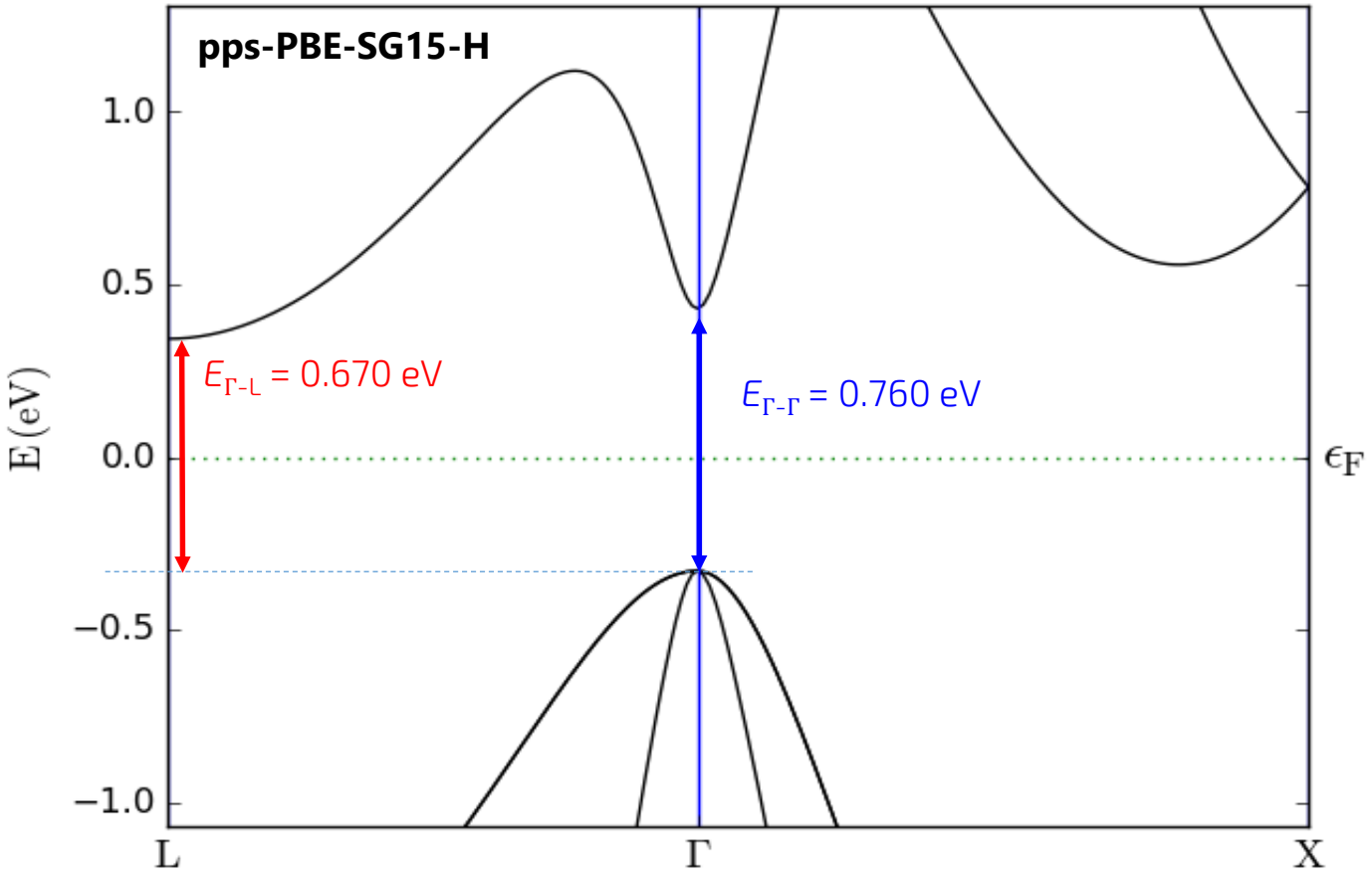
Pseudopotential projectors shifts (PPS) method

- Inspired by empirical pseudopotentials but still operates within the full DFT framework
- Tunable parameters are added to the pseudopotential projectors or each angular momentum of the core electron system (unlike +*U* which operates on the valence electrons)

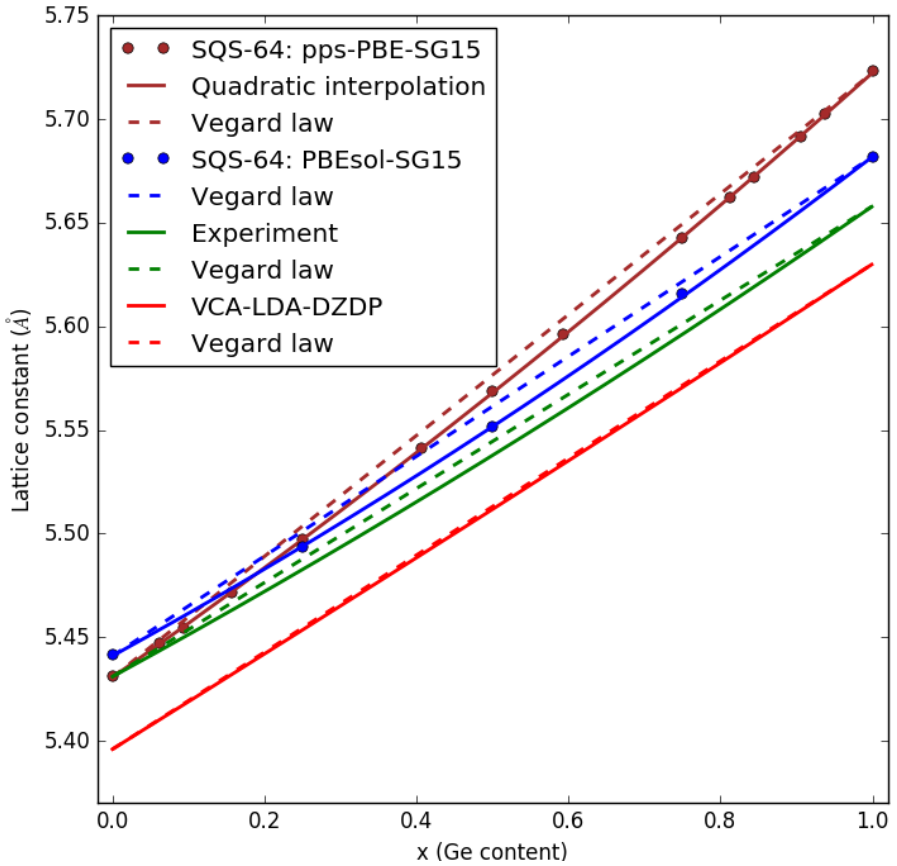
$$V_{\mathrm{ps}}(\mathbf{r}) = V_{\mathrm{ps}}^{\mathrm{loc}}(\mathbf{r}) + \sum_{\alpha\beta} |\alpha\rangle [V_{\alpha\beta} + U_{\alpha\beta}] \langle\beta|,$$

- Influences observables such as lattice constants and band gaps
- Shifts are determined by fitting observables to experiments
- Appears to mimic a scissors operator, leaving e.g. effective masses in Si unchanged
- So far tested mainly for Si and Ge – and SiGe
  - Possible to fit your own parameters

Band structure of Ge



Compositional dependence of the lattice parameter



$a_{VCA}(x) = (5.396 + 0.2288\,x + 0.00529\,x^2)$ Å

$a_{SQS\text{-}pps\text{-}PBE}(x) = (5.431 + 0.2572\,x + 0.03439\,x^2)$ Å

$a_{SQS\text{-}PBEsol}(x) = (5.441 + 0.2017\,x + 0.03915\,x^2)$ Å

$a_{exp}(x) = (5.431 + 0.20\,x + 0.027\,x^2)$ Å

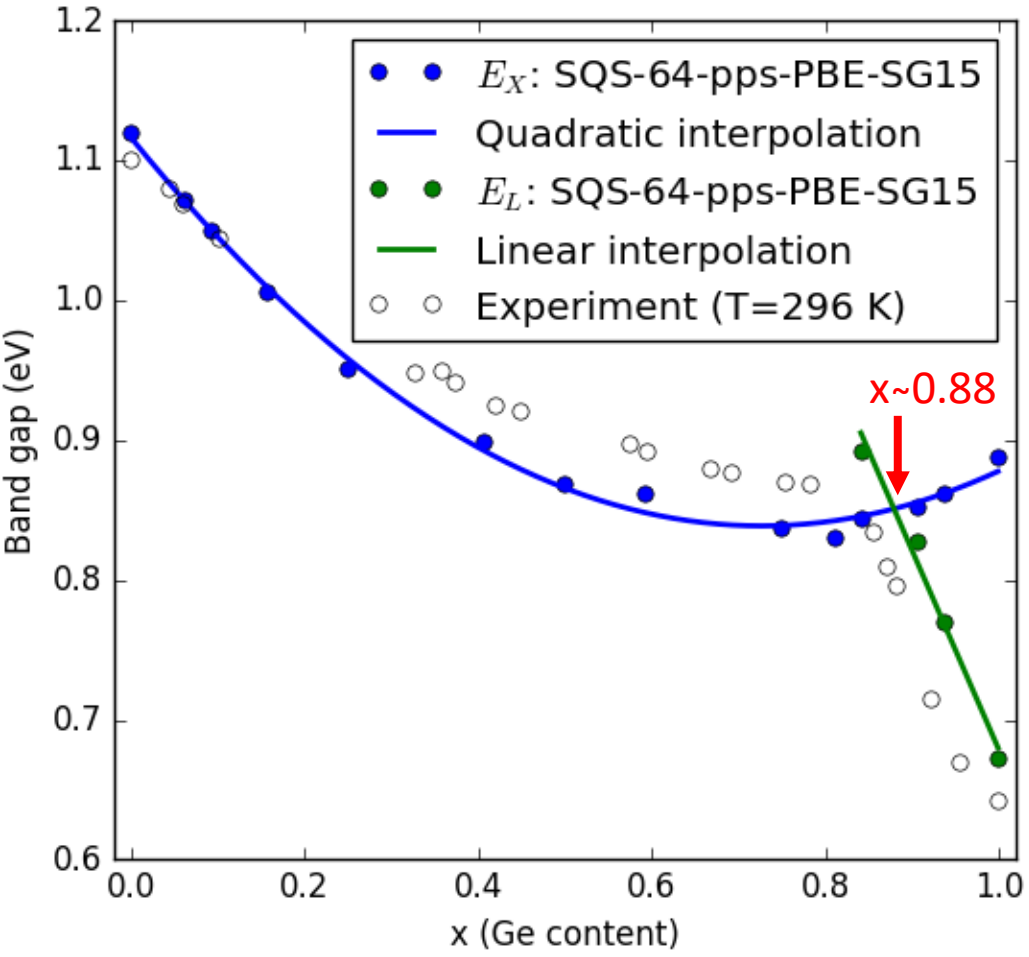
http://www.ioffe.ru/SVA/NSM/Semicond/SiGe/basic.html

The lattice constants were calculated by total energy calculations (geometry optimization) that included volume and ion relaxation of the SQS-64 structures generated for different SiGe compounds.

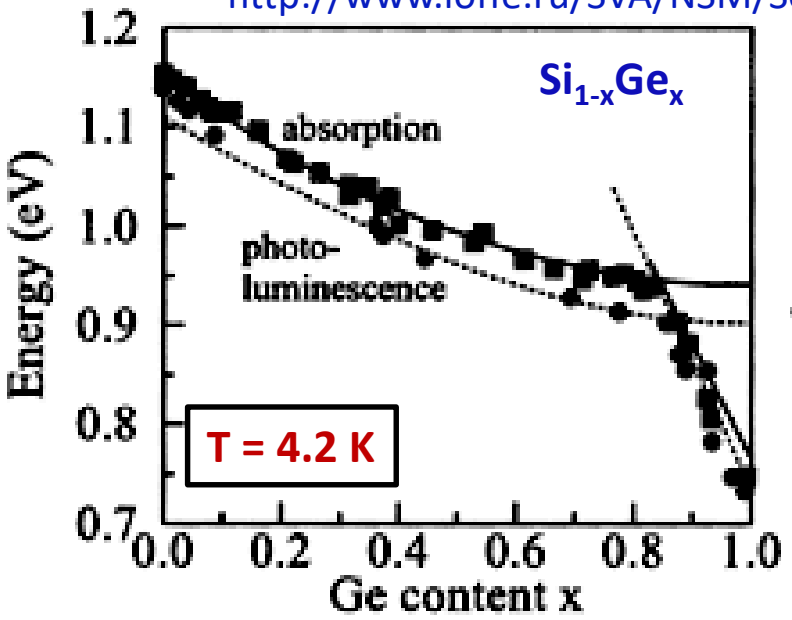
Conclusion: the downward compositional bowing of 0.039 (0.034) Å for the $Si_{1-x}Ge_x$ alloy lattice constant calculated in the ATK using the PBEsol-SG15 (pps-PBE-SG15) approach combined with the SQS modeling of random alloys agrees well with the experimentally measured bowing of 0.027 Å.

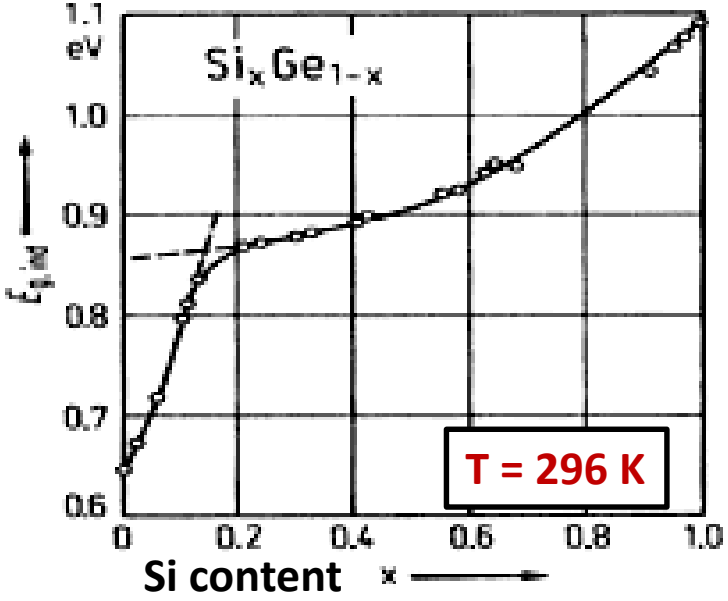
The compositional bowing calculated using the VCA approach is 0.005 Å, meaning that it is strongly underestimated. This is because the VCA does not account for the effect of ion relaxation on the structural properties of alloys.

Compositional dependence of the band gap energy for $Si_{1-x}Ge_x$ alloys



http://www.ioffe.ru/SVA/NSM/Semicond/SiGe/bandstr.html





$E_{gap}(x) = (1.12 - 0.764\,x + 0.525\,x^2)$ Å for $x < 0.88$

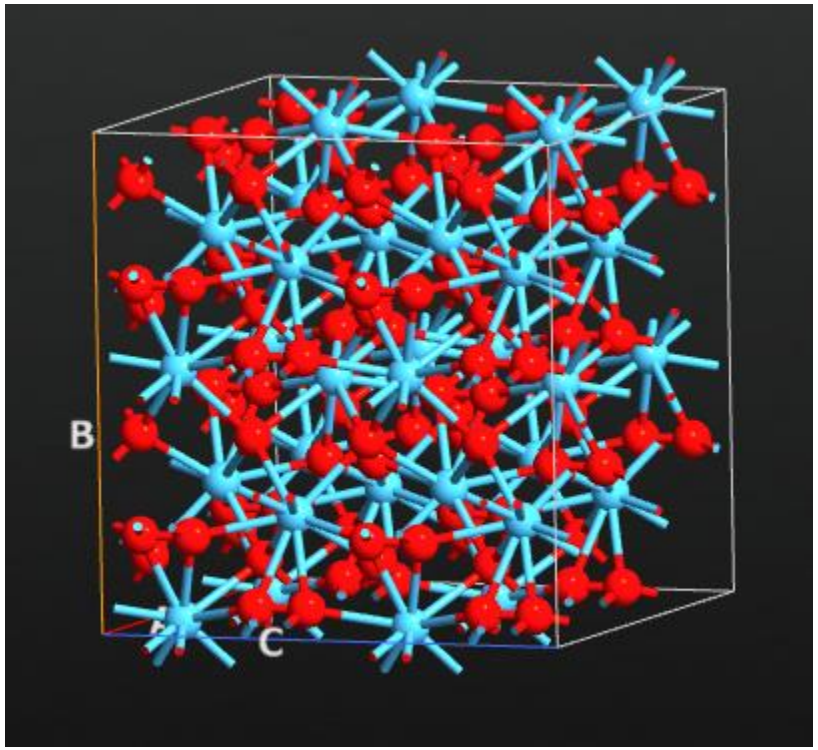
$(2.104 - 1.425\,x)$ Å for $0.88 < x < 1$

Conclusions: the ATK pps-PBE-SG15 ab initio approach combined with SQS-64 modeling of random alloys predicts that the *X-L* transition of the indirect band gap in $Si_{1-x}Ge_x$ alloys occurs at x^*~0.88, in agreement with experiments (x^*~0.85).

The calculated compositional dependence if the $Si_{1-x}Ge_x$ band gap agrees well (within 0.03 eV) with the experimental data. Both the ATK calculations and measurements show downward compositional bowing (no bowing) of the gap at $x<x^*$ ($x>x^*$).

Phonon calculations of large supercells

- How to calculate thermal properties due to defects?
- We need to compute the phonon DOS/spectrum, i.e. first we need the dynamical matrix
- Minimal cell is a 3x3x3 repetition
- Take HfO2 (2x2x2 supercell) with an oxygen vacancy
  - 762 calculations (6 displacements per atom), each containing 127 x 3x3x3 = 3429 atoms
  - Ok for classical potentials, but for interstitials, and complex materials you need DFT = extremely time-consuming



Simplified supercell method, or Wigner-Seitz scheme

- ATK 2017 introduces an approximation for obtaining the dispersion of vibrational eigenmodes with a force calculation of the unit cell only (repetitions = [1,1,1] or “the poor man’s frozen phonon calculation”)
- Exact in the limit of large supercells, but has good accuracy already for small cells, esp. for acoustic phonon DOS

Disregard force contributions to the density matrix between atoms > half the unit cell size from each other

DynamicalMatrix

class **DynamicalMatrix** *(configuration, calculator=None, repetitions=None, atomic_displacement=None, acoustic_sum_rule=None, symmetrize=None, finite_difference_method=None, constraints=None, constrain_electrodes=None, use_equivalent_bulk=None, max_interaction_range=None, force_tolerance=None, processes_per_displacement=1, log_filename_prefix='displacement_', use_wigner_seitz_scheme=None, repeats=None)*

Constructor for the **DynamicalMatrix** object.

Parameters:
- **configuration** (`BulkConfiguration` | `MoleculeConfiguration` | `DeviceConfiguration`) – The configuration for which to calculate the dynamical matrix.

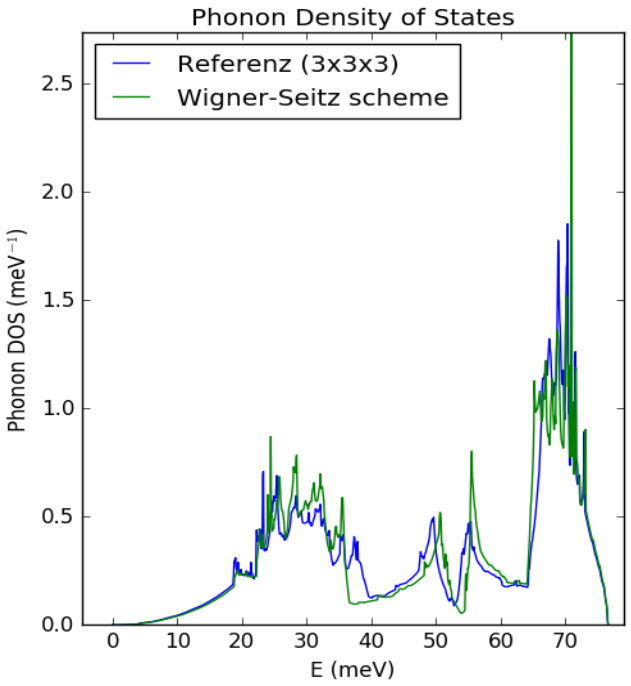
- **use_wigner_seitz_scheme** (*bool*) – Control if the real space Dynamical Matrix should be extended according to the Wigner Seitz construction.
  Default: `True`

The Wigner-Seitz construction ensures that the phonon spectrum at the Γ-point is preserved. Hence, a separate Γ-point calculation is not necessary.

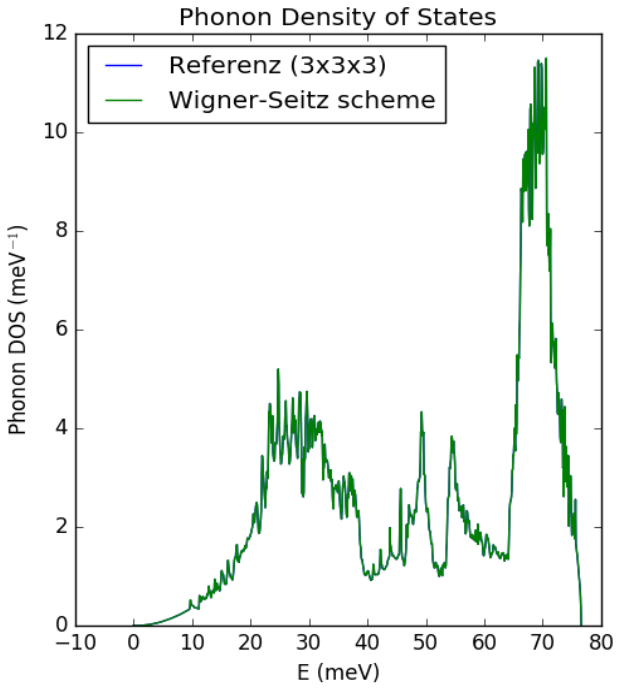
Example 1

- Si (simple cubic supercell)
- Classical potential with a finite range
- The approximation becomes exact for a large enough supercell

8 atoms / unit cell

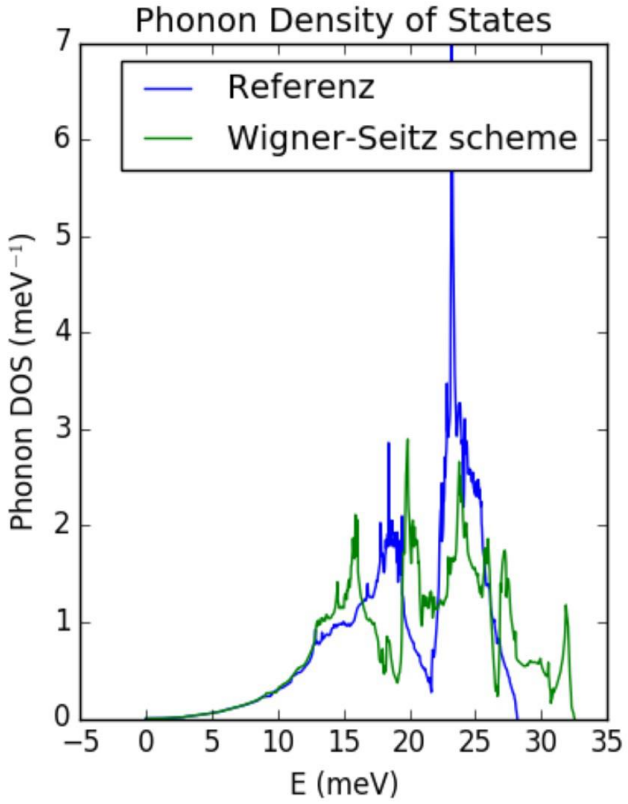


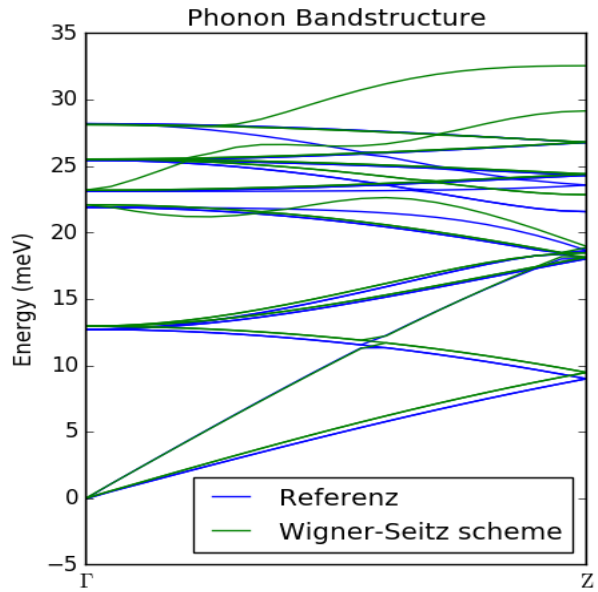
64 atoms / unit cell



Example 2

- NaCl, 8 atoms
- DFT – long range effects are prevalent
- Some deviation seen at higher energy, very accurate below 12 meV
- 50x speedup
  - Full 3x3x3 repetition: 1.5 hours
  - Wigner-Seitz scheme: 2 minutes
- Expect a 64-atom supercell to be very accurate

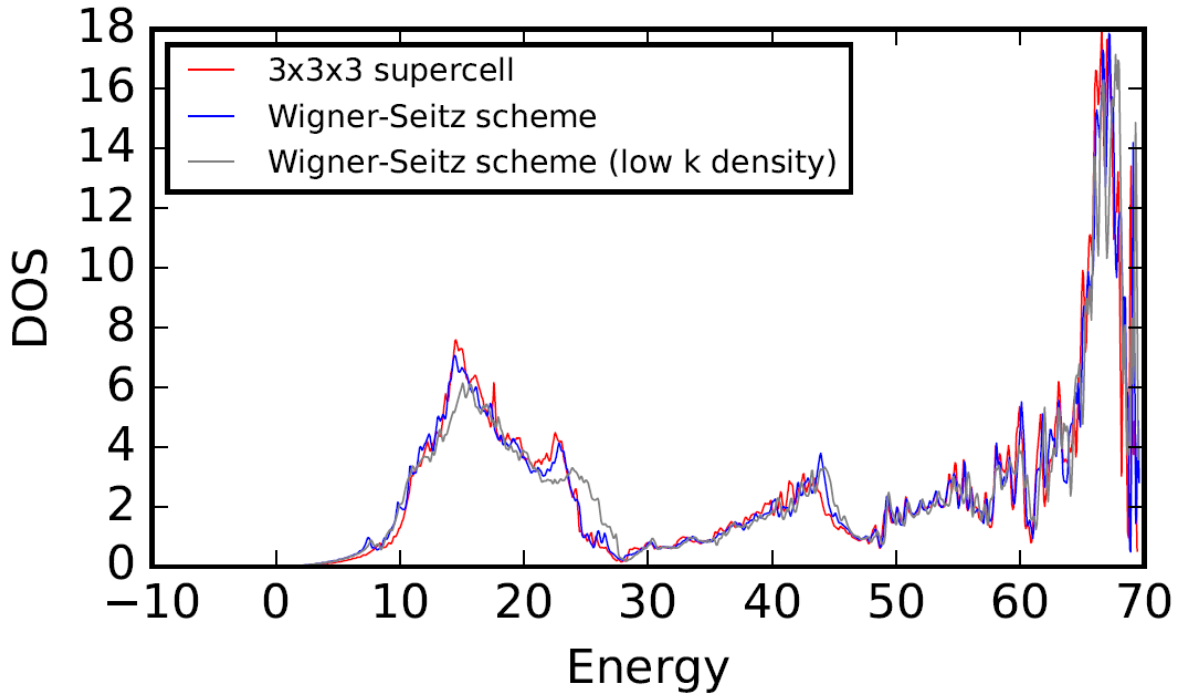


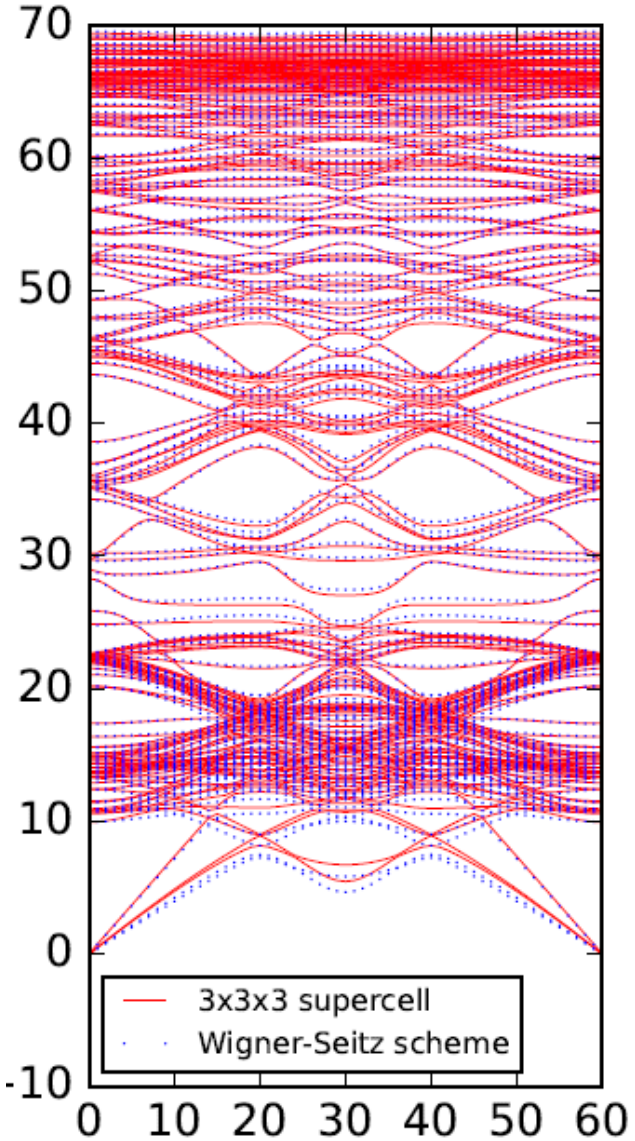


Example 3

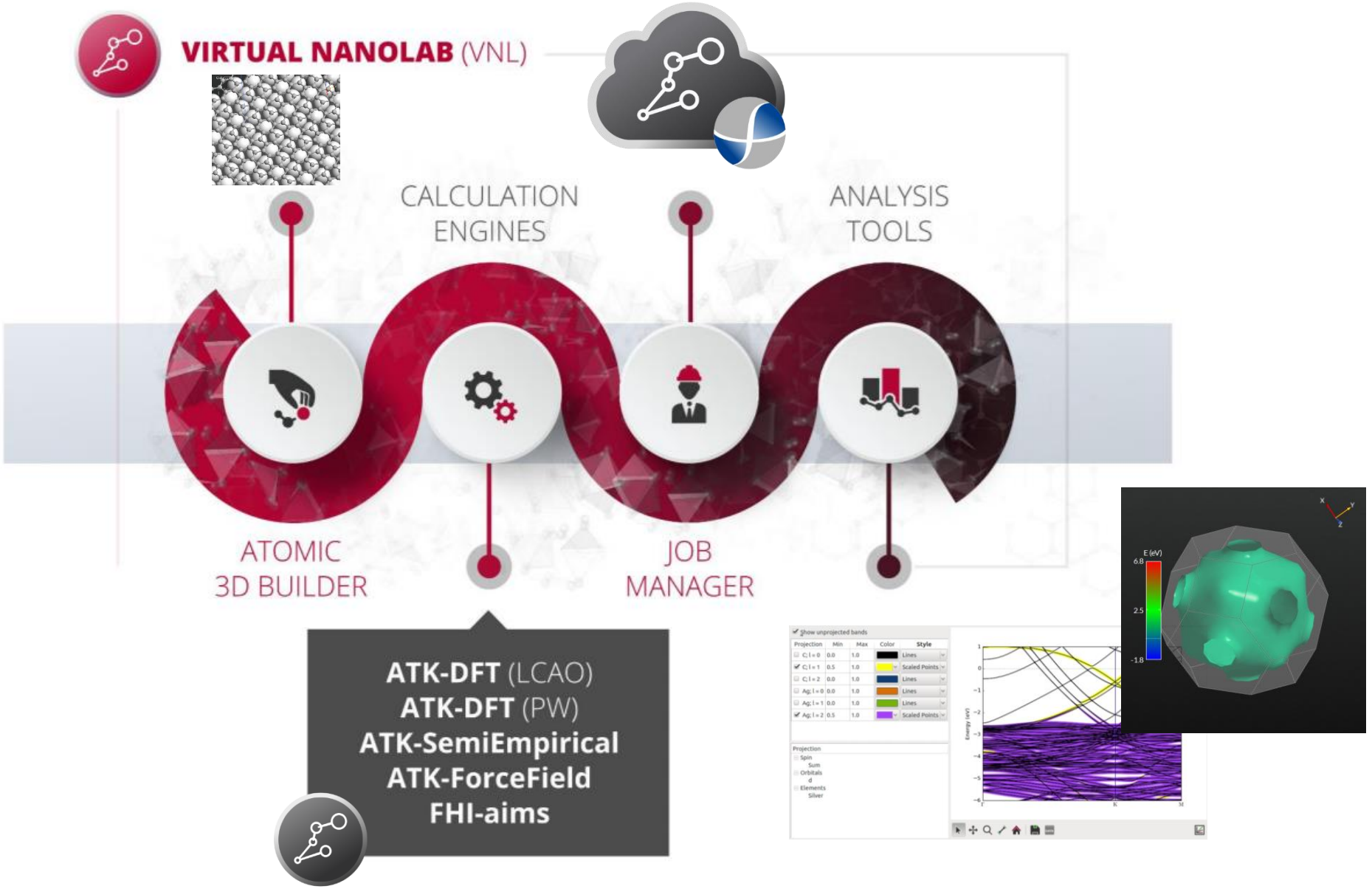
- Si supercell with one vacancy (63 atoms)
- DFT, minimal basis set (SingleZeta)
- W-Z = 3x3x3 k-points (low-k = 1x1x1)
- 300x speedup

	3x3x3 supercell	simplified scheme
time	9 days	43 minutes

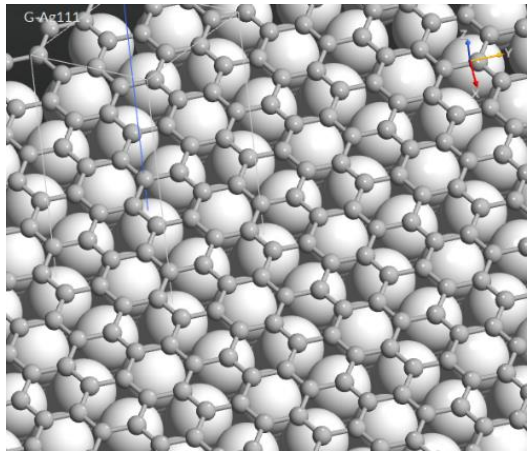




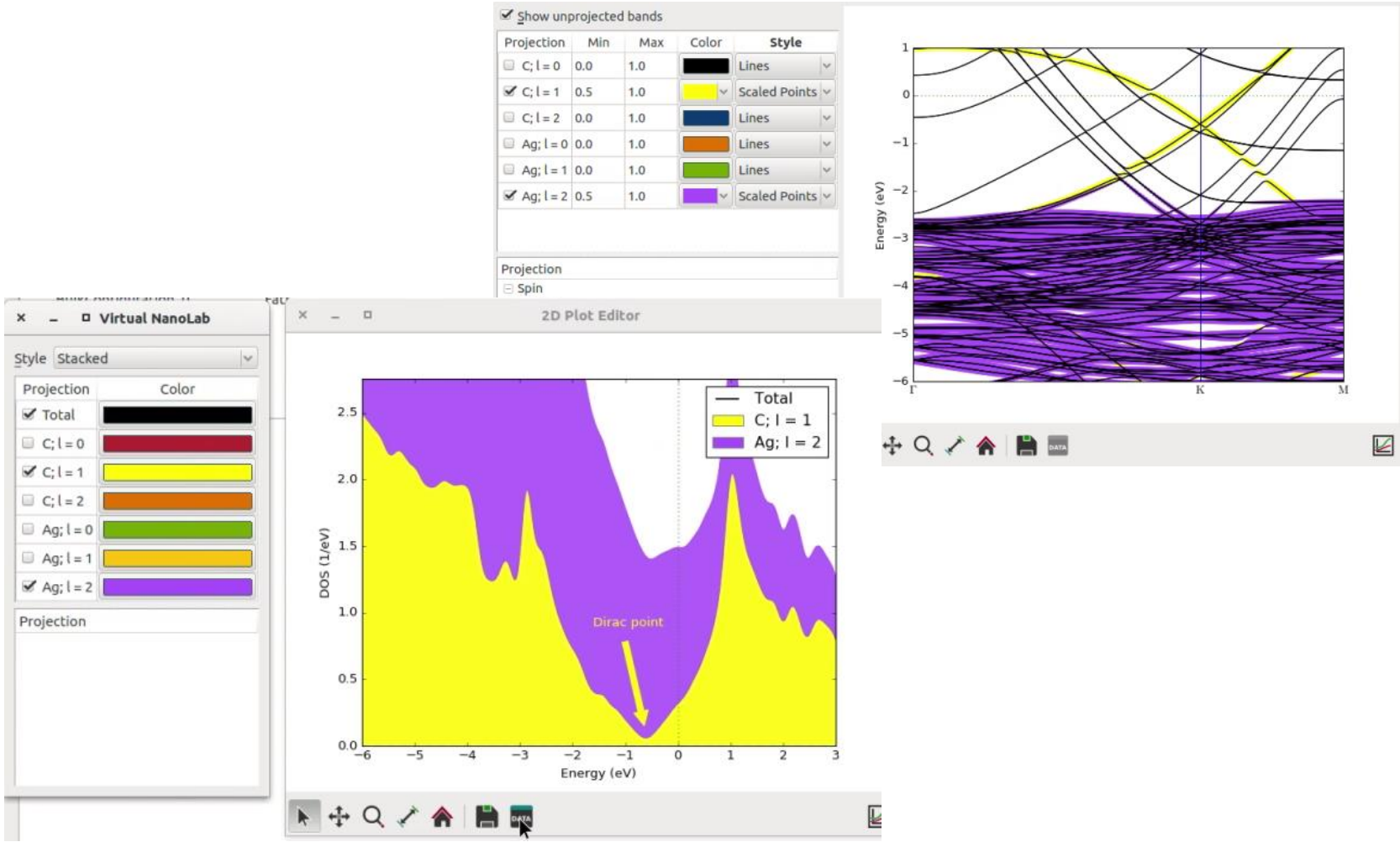
VNL/ATK platform workflow



Fat band structure and projected density of states

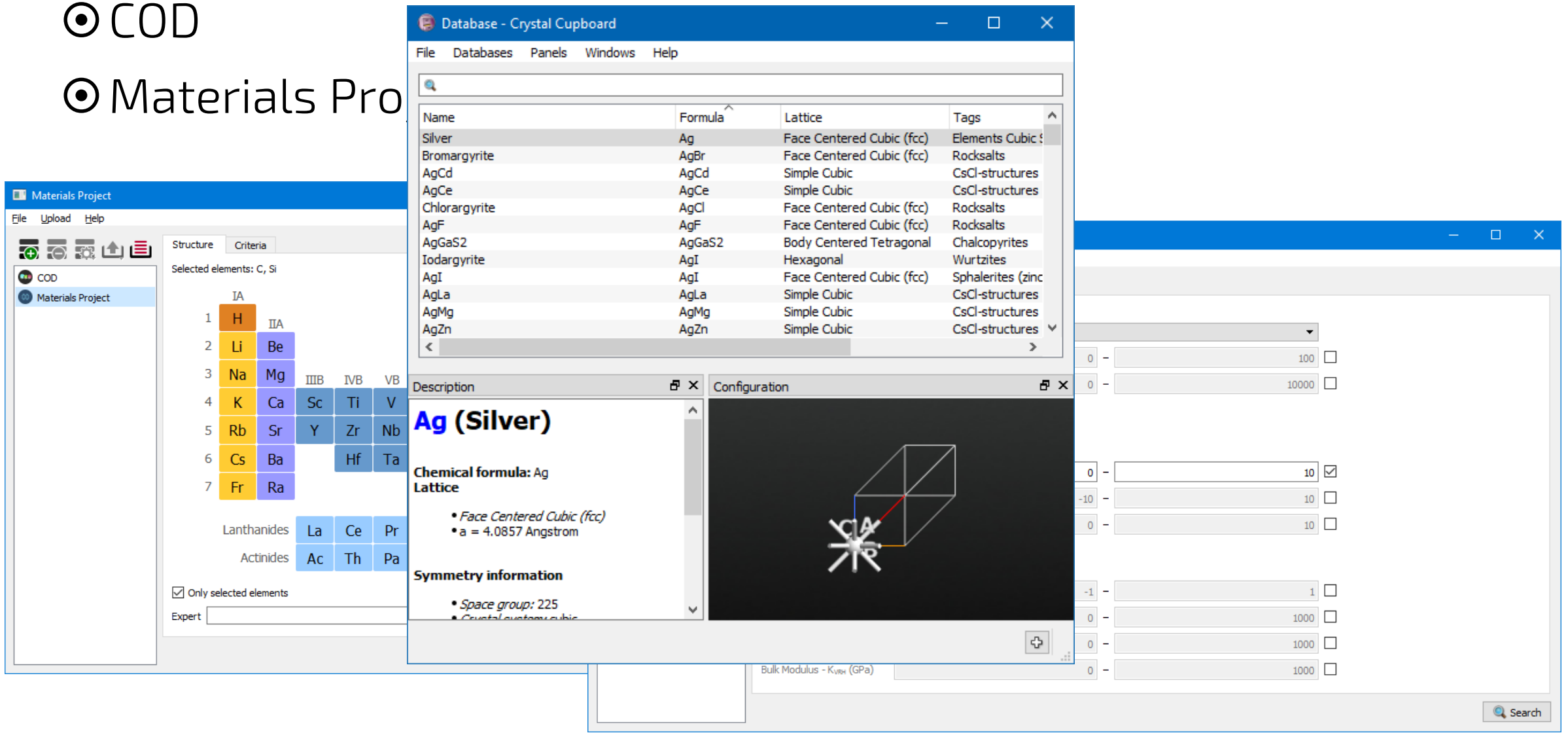


Graphene on Ag(111)



Databases

- COD
- Materials Pro

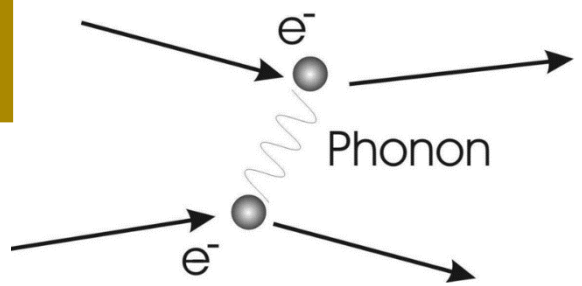


Electron-phonon interaction

ELECTRONS
(band structure, transmission)
DFT, DFTB, Slater-Koster

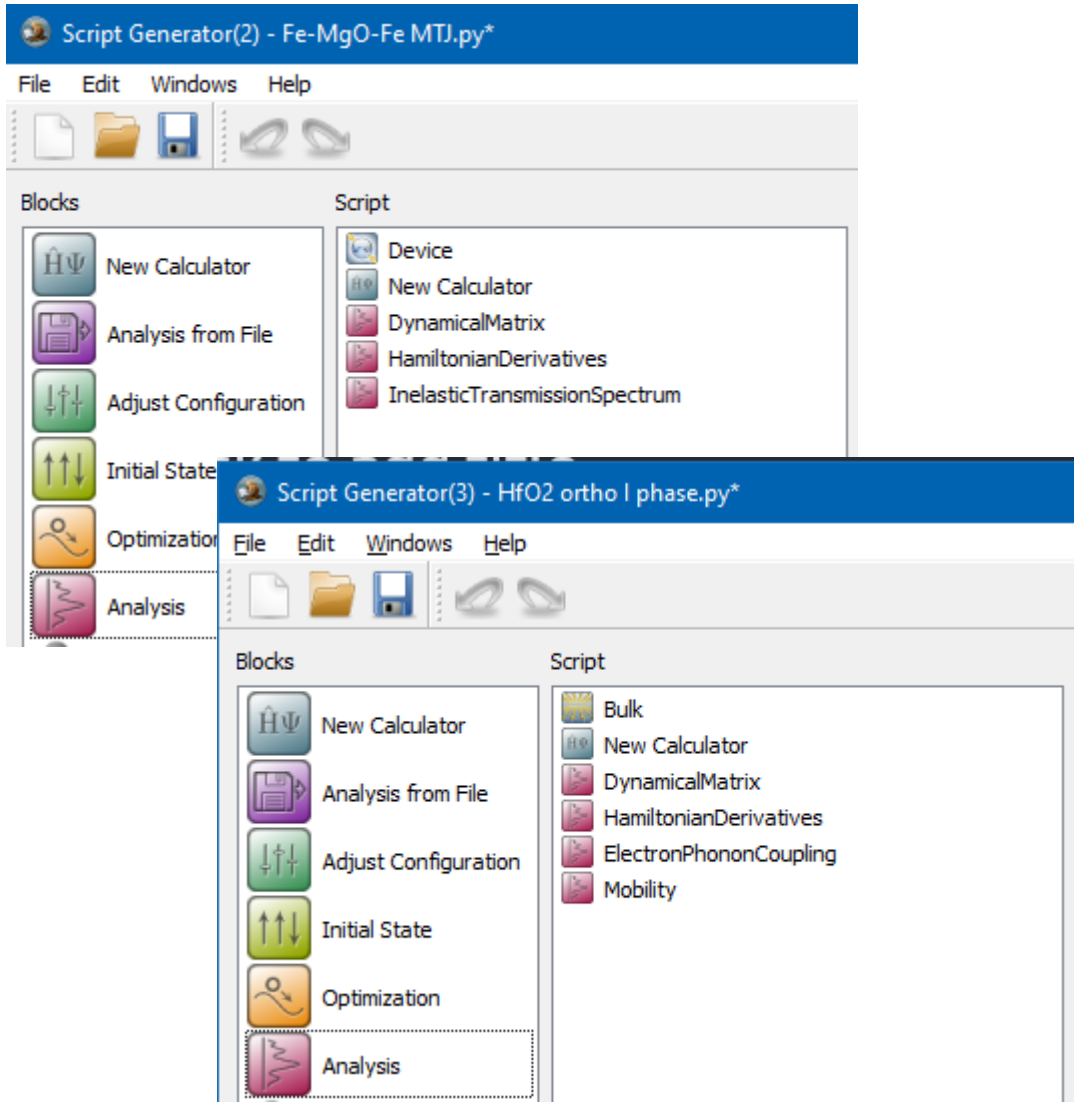
PHONONS
(dynamical matrix)
DFT, DFTB, Classical potentials

EL-PH COUPLING
(mobility, inelastic current)



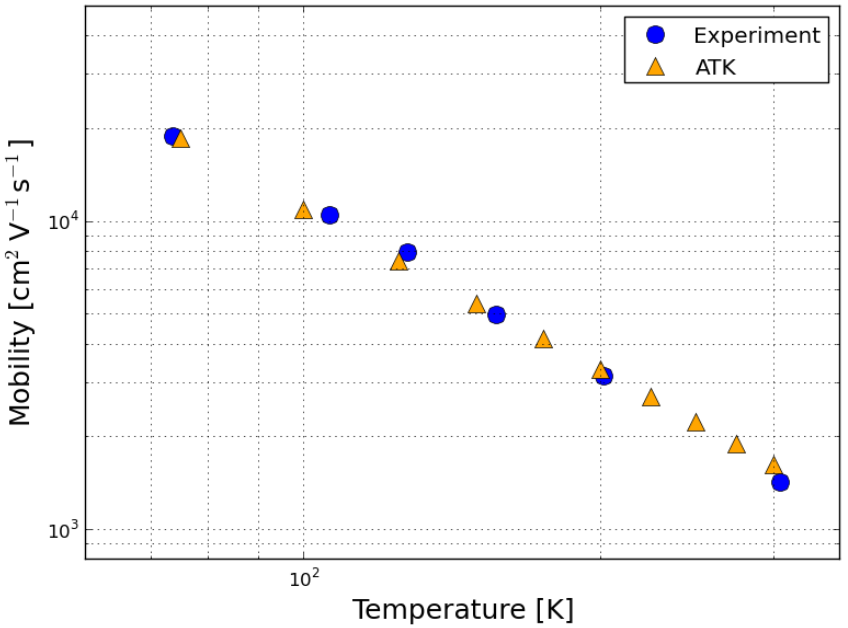
Complex calculation

- Requires several ingredients
  - Dynamical matrix
  - dH/dR
  - For bulk:
    - El-ph coupling
    - Deformation potentials
    - Boltzmann eq. -> μ
  - For devices:
    - XLOE/LOE -> Inelastic transmission spectrum -> I(V)
- Different methods can be used for electrons and phonons
  - DFT, classical potentials, DFTB, tight-binding
- Different parallelization schemes may be required for each step to perform optimally



Improvements in ATK 2017

- Significantly lower memory requirement by storing all matrices as sparse
  - For one calculation it was benchmarked to go from 800 GB to 1.3 GB!
- New option for mobility: constant relaxation time (similar to Boltztrap); tau can be provided, e.g. from experiments, but can also be computed on-the-fly
- Gain 10-100x in performance by grouping (summing) all phonon modes in an energy range, as an approximation
- 1,000-100,000x faster if the device is homogeneous along the transport direction (like a long, simple nanowire, nanotube, Si p-n junction, or 2D slab)
  - Only need to calculate the dynamical matrix and dH/dR for the electrode



http://docs.quantumwise.com/tutorials/inelastic_current_in_si_pn_junction

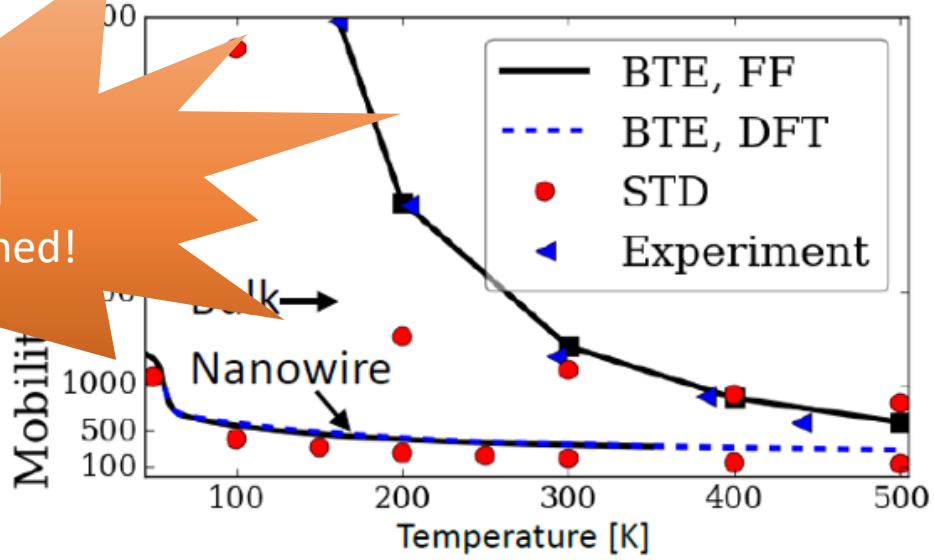
Special thermal displacement (STD) approximation

- Capture the effect of phonon scattering on the I-V curve by creating a single distorted atomic configuration based on a canonical average over all phonon modes
- Reduces the complete electron-phonon coupling calculation to
  - Evaluation of the dynamical matrix of the central reg
  - A single device calculation each bias (and temperature)

$$\mathcal{T}_{STD}(E,T) = \mathcal{T}_0(E) - \sum_{\lambda} \frac{\partial \mathcal{T}(E,\{\mathbf{u}_\lambda\})}{\partial \mathbf{u}_\lambda} s_\lambda (-1)^{\lambda-1} \sigma_\lambda(T)$$
$$+\frac{1}{2}\sum_{\lambda\lambda'} \frac{\partial^2 \mathcal{T}(E,\{\mathbf{u}_\lambda\})}{\partial \mathbf{u}_\lambda \partial \mathbf{u}_{\lambda'}} s_\lambda s_{\lambda'} (-1)^{\lambda+\lambda'-2} \sigma_\lambda(T)\sigma_{\lambda'}(T) + \mathcal{O}(\sigma^3)$$

Dedicated webinar planned!

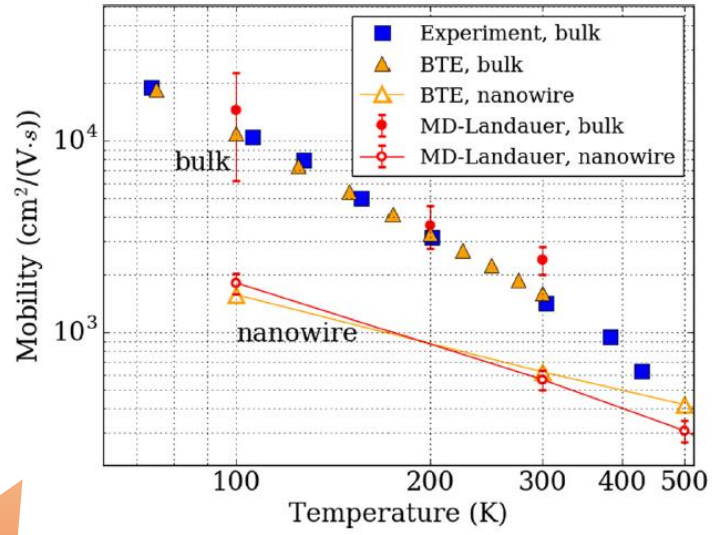
Example: Si nanowire

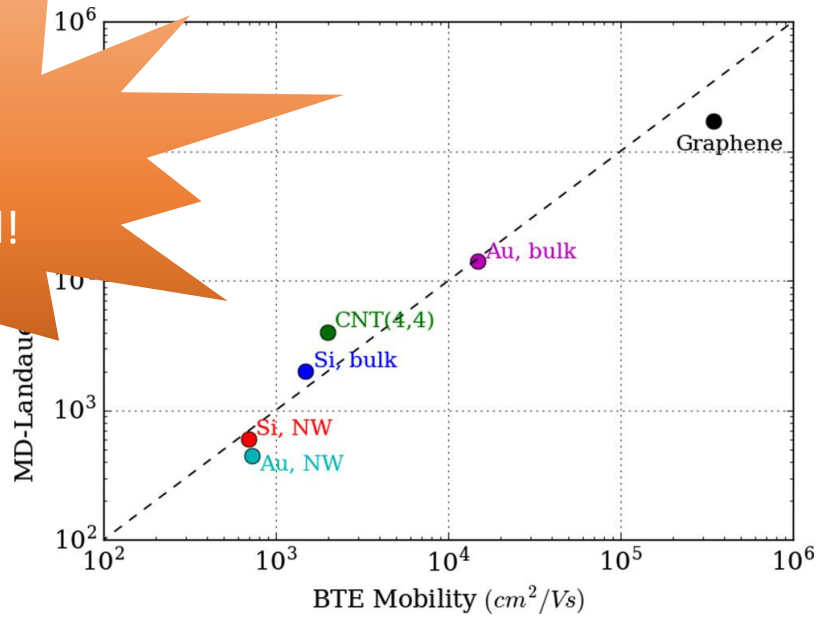


For details see arXiv:1706.09290

Molecular dynamics + Landauer approximation

- Capture the effect of phonon scattering via molecular dynamics
- Average the transmission spectra of MD configuration snapshots in time
  - Computed with the usual Landauer approach
  - Mobility is obtained by making the central region longer and longer
- Example: phonon contribution to grain boundary scattering in meta
- Avoids ever computing the dynamical matrix
  - But requires a classical potent MD part

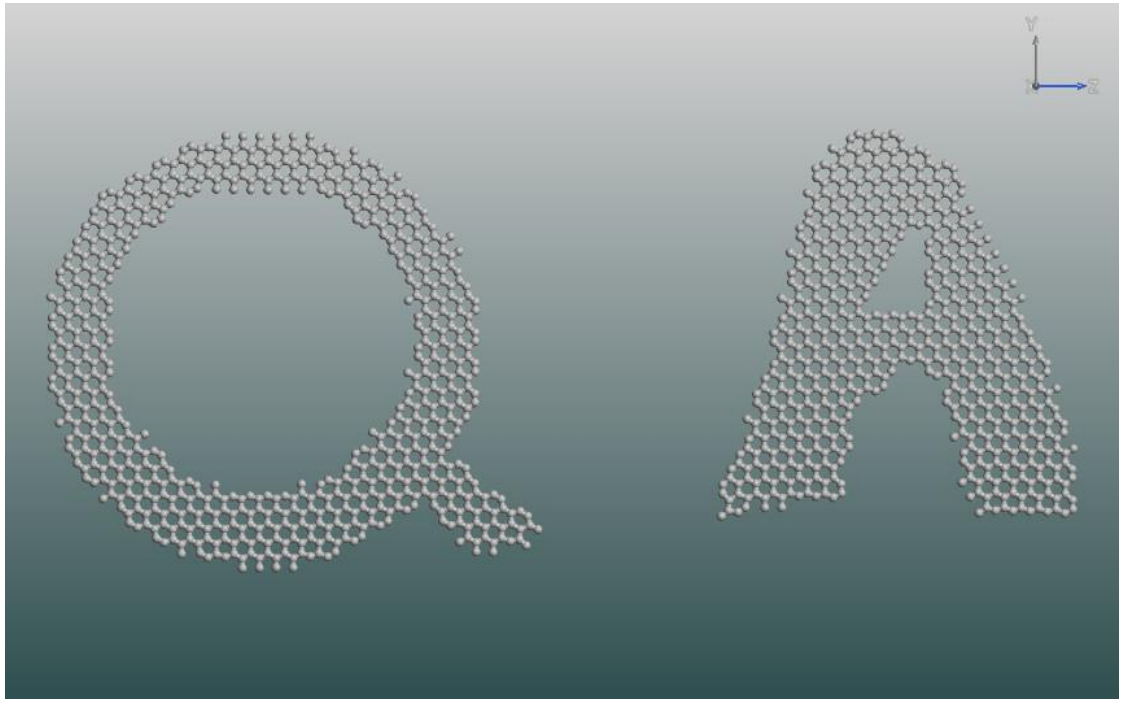




Dedicated webinar planned!

For details see PRB 95, 245210 (2017)

Questions?



Thank You!

Quantum Wise