THE UNIVERSITY OF ARIZONA

Updates to the FHI-aims Python Environments

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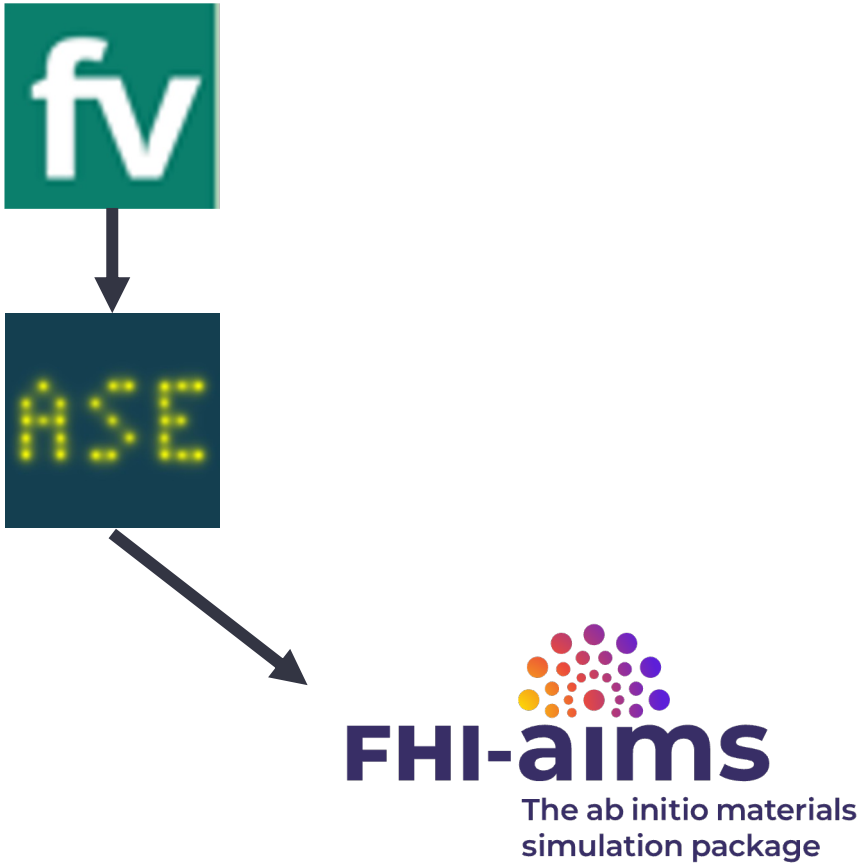
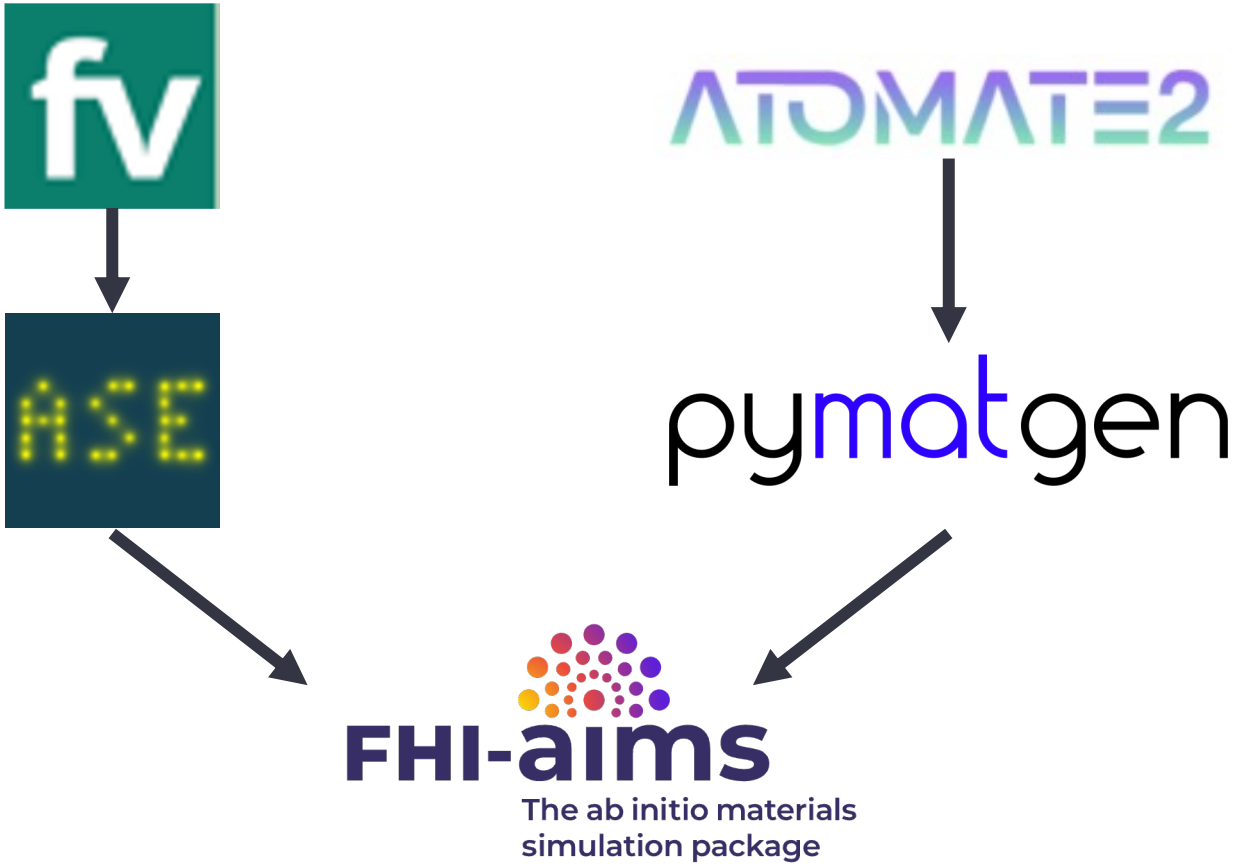
Maintaining the Python Interfaces



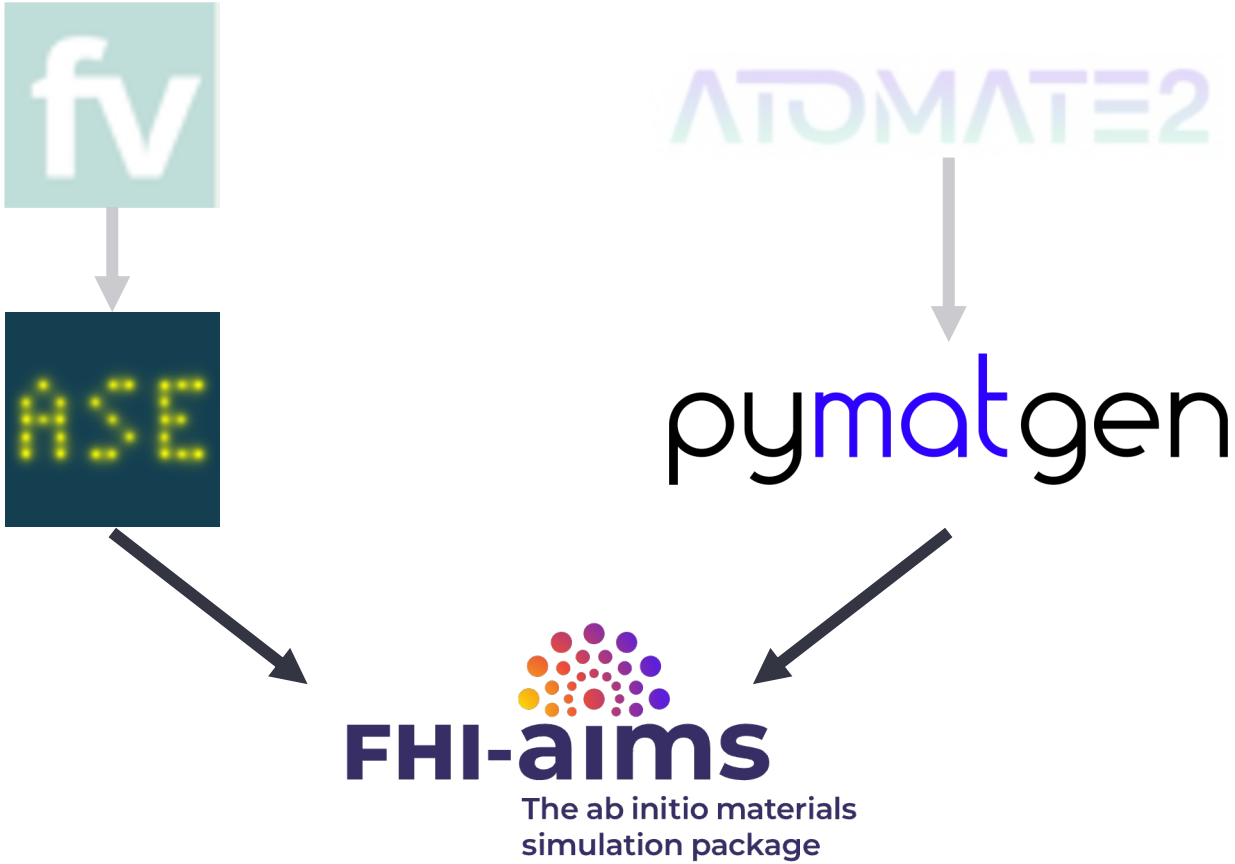
Atomate2 Workflows

Workflow	System	ASE	FHI-AIMS
Geometry optimization	Both	✓	✓
Static	Both	✓	✓
Dielectric	Periodic	—	—
Polarization	Periodic	—	—
Electronic band structure	Periodic	—	✓
Bond analysis workflow with LOBSTER	Periodic	—	—
Excited states (GW-BSE)	Periodic	△	✓
Ab initio molecular dynamics	Periodic	✓	△
Force field molecular dynamics	Periodic	✓	✓
Elastic constants	Periodic	△	✓
Harmonic phonons	Periodic	△	✓
Equation of state	Periodic	△	✓
Electron–phonon	Periodic	—	—
Grüneisen	Periodic	—	△
Matpes	Periodic	—	—
Quasiharmonic approximation for phonons	Periodic	—	△
Anharmonic phonons	Periodic	△	○
MPMorph	Periodic	△	△
Magnetic ordering	Periodic	△	✓
Adsorption	Periodic	△	△
Point defect	Periodic	△	○
Anharmonicity quantification	Periodic	△	✓
Electrode discovery	Periodic	△	—
Ferroelectric	Periodic	△	—
Materials project	Periodic	—	—
Amset	Periodic	—	—
Frequency flatterning optimizer workflow	Molecular	—	—
Classical molecular dynamics workflow	Molecular	✓	—

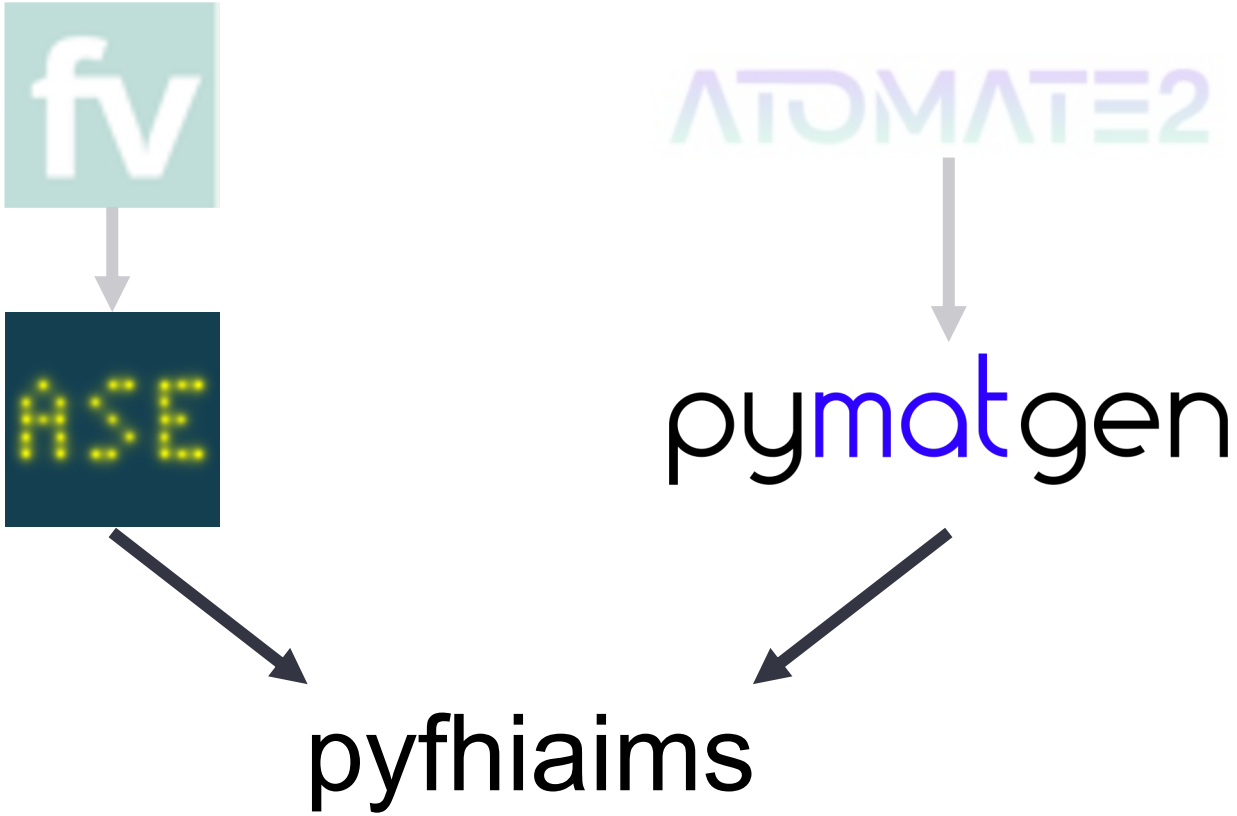
Maintaining the Python Interfaces



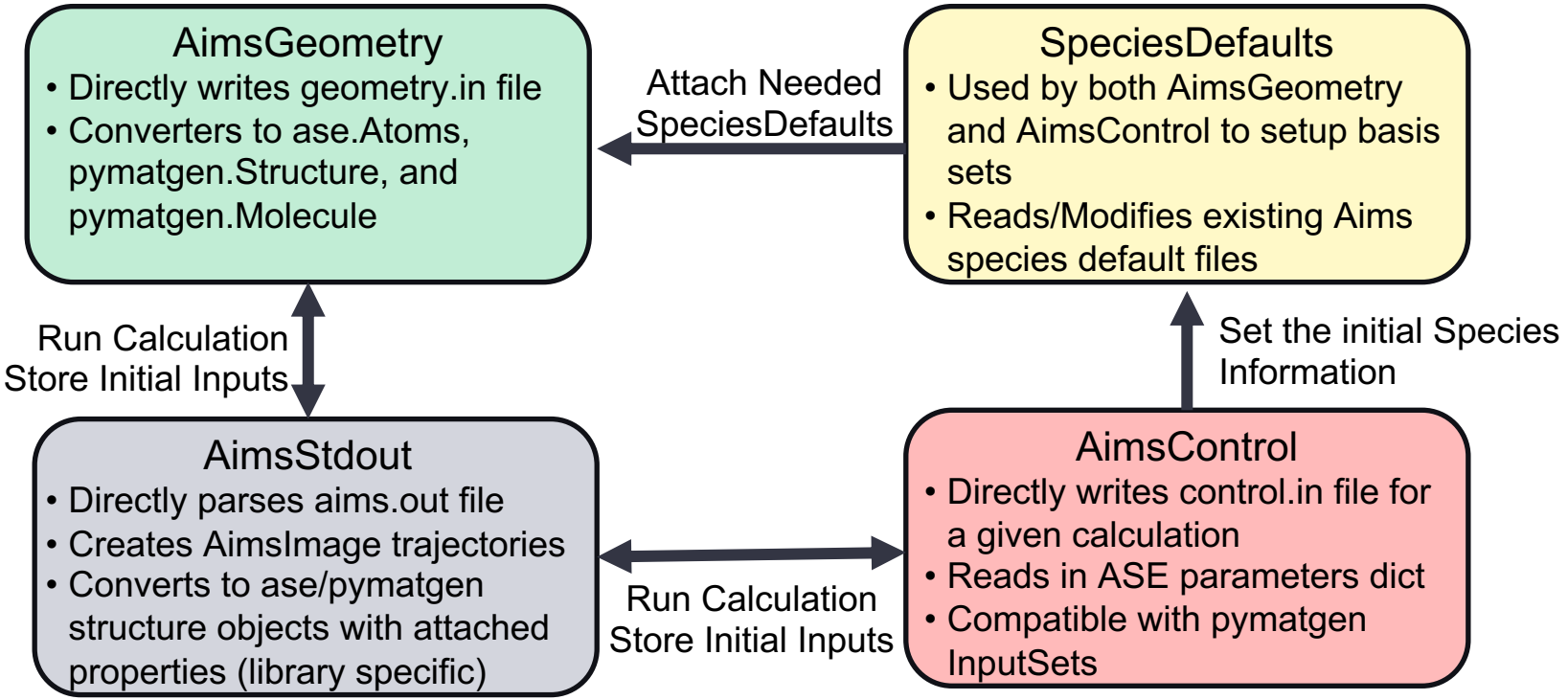
Two Interfaces Containing Basically the Same Information



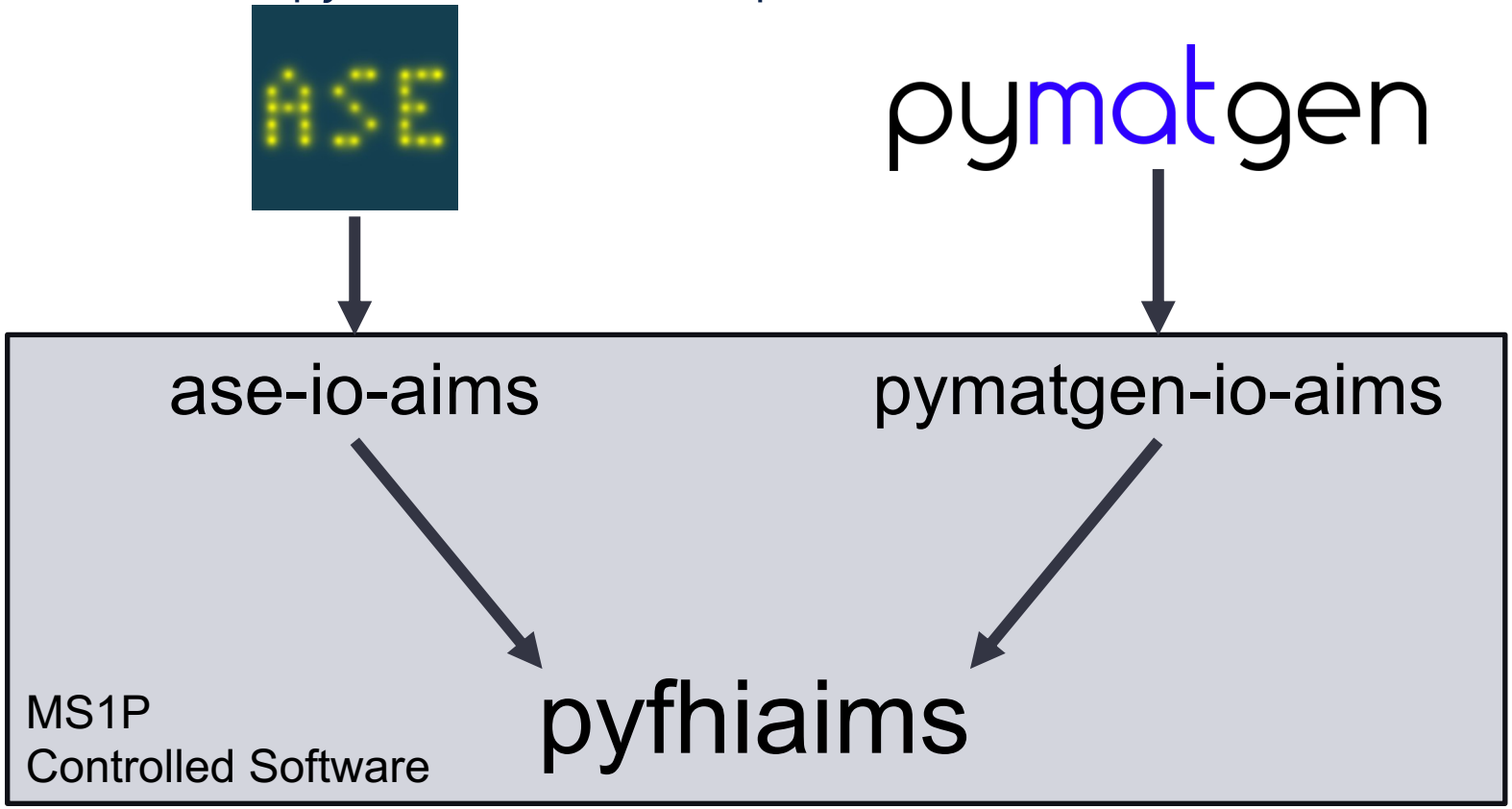
Creating a single interface to FHI-aims



How pyfhiaims works

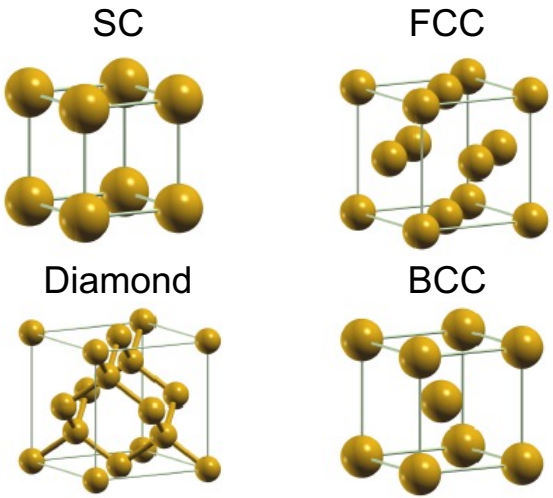


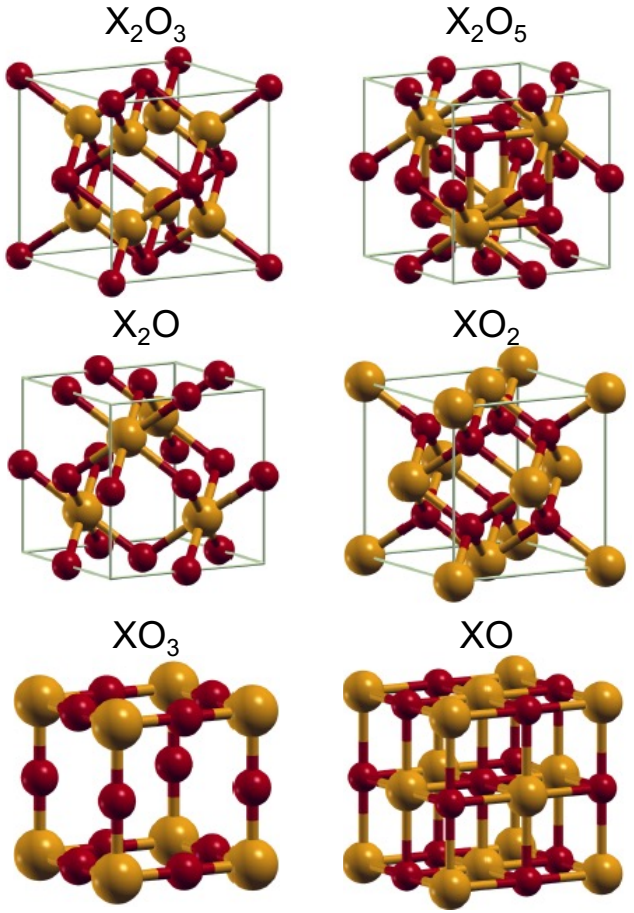
New FHI-aims python environment plan



Applying this for benchmarking

Benchmarking DFT Codes for Solids





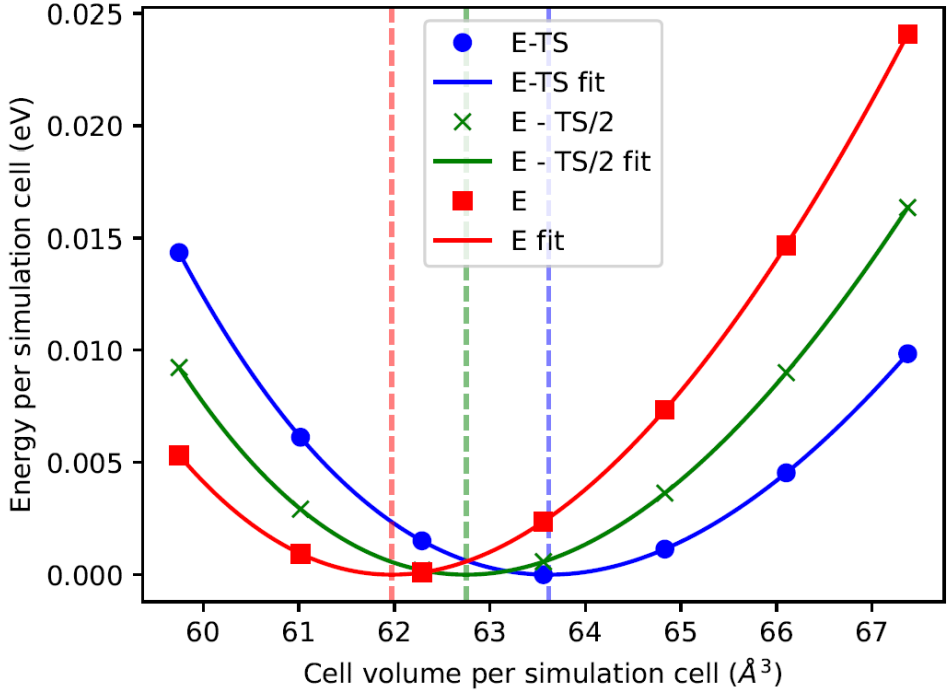
Bosoni, E.; *et al. Nat. Rev. Phys.* **2024.** *6.* 45

Benchmark Target: Birch-Murnaghan Equation of State

$$E(V) = E_0 + \frac{9V_0B_0}{16}\left\{\left[\left(\frac{V_0}{V}\right)^{\frac{2}{3}} - 1\right]^3 B_1 + \left[\left(\frac{V_0}{V}\right)^{\frac{2}{3}} - 1\right]^2 \left[6 - 4\left(\frac{V_0}{V}\right)^{\frac{2}{3}}\right]\right\}$$

$$\langle f \rangle = \frac{1}{V_\mathrm{M} - V_\mathrm{m}} \int_{V_\mathrm{m}}^{V_\mathrm{M}} f(V)\mathrm{d}V$$

$$\varepsilon(a,b) = \frac{\left\langle [E_a(V) - E_b(V)]^2 \right\rangle}{\sqrt{\left\langle [E_a(V) - \langle E_a \rangle]^2 \right\rangle \left\langle [E_b(V) - \langle E_b \rangle]^2 \right\rangle}}$$



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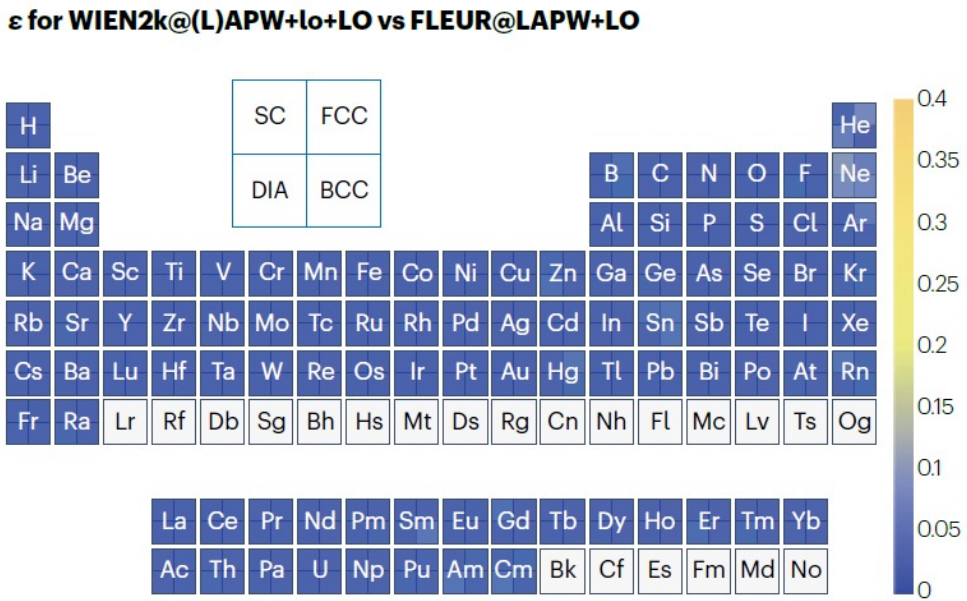
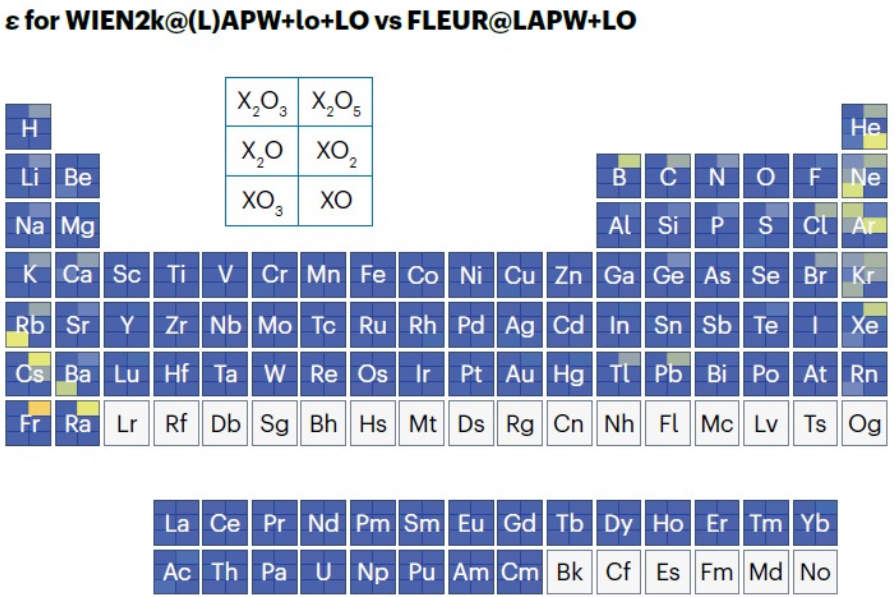
Previous demonstration of strong agreement between all-electron codes





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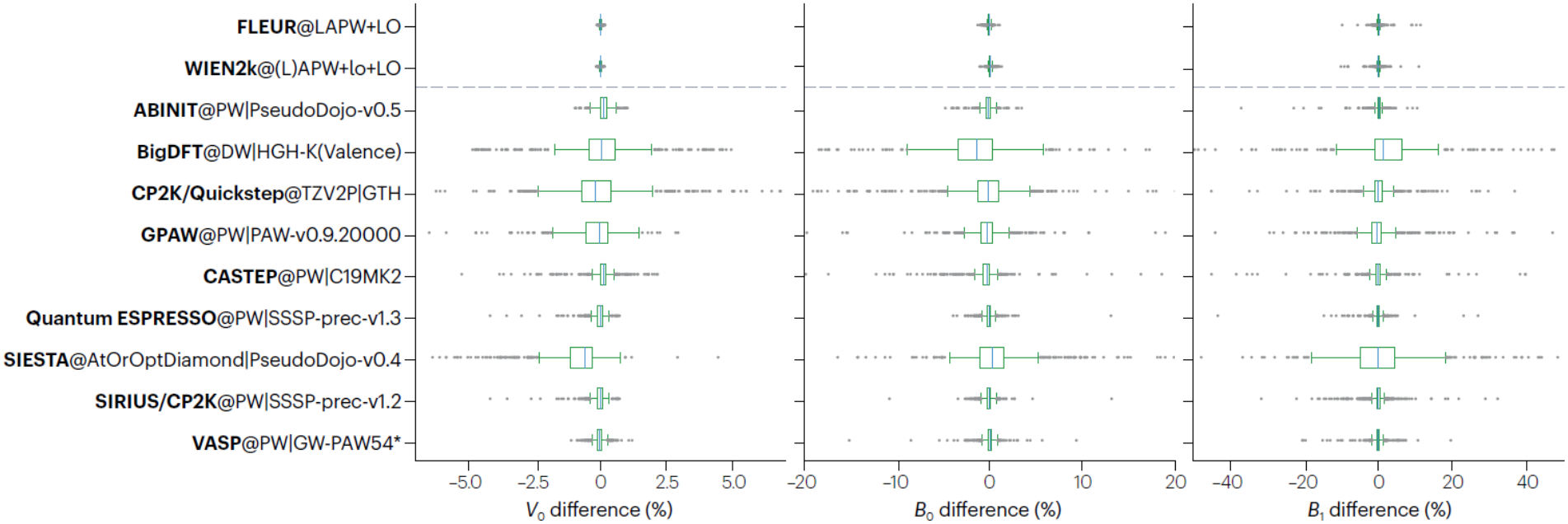
Pseudopotentials show larger disagreements



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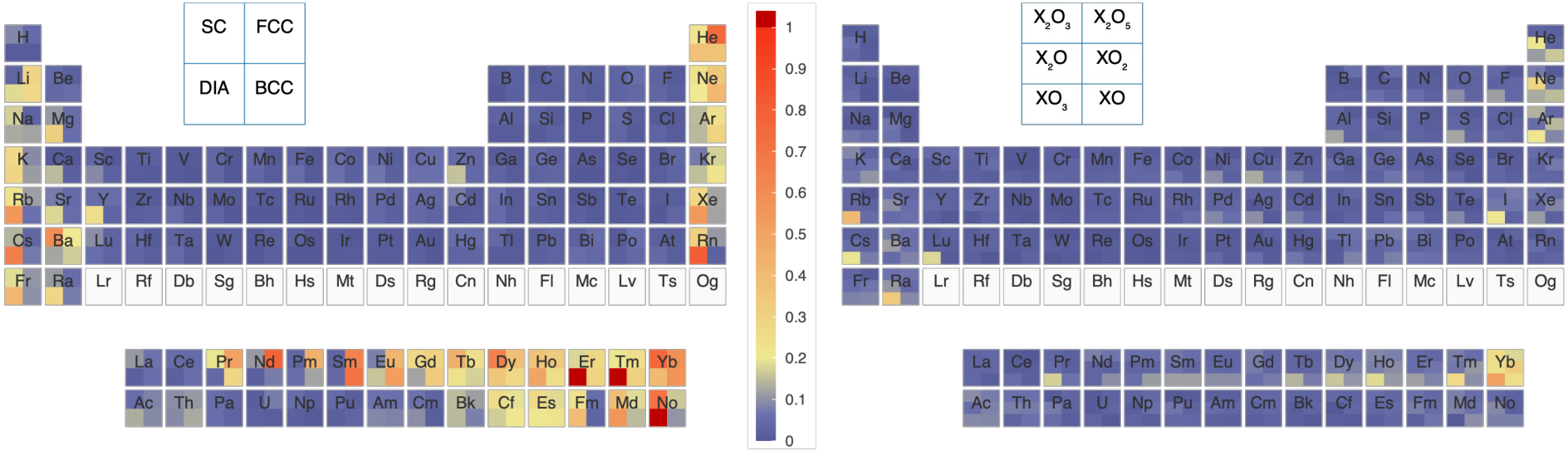
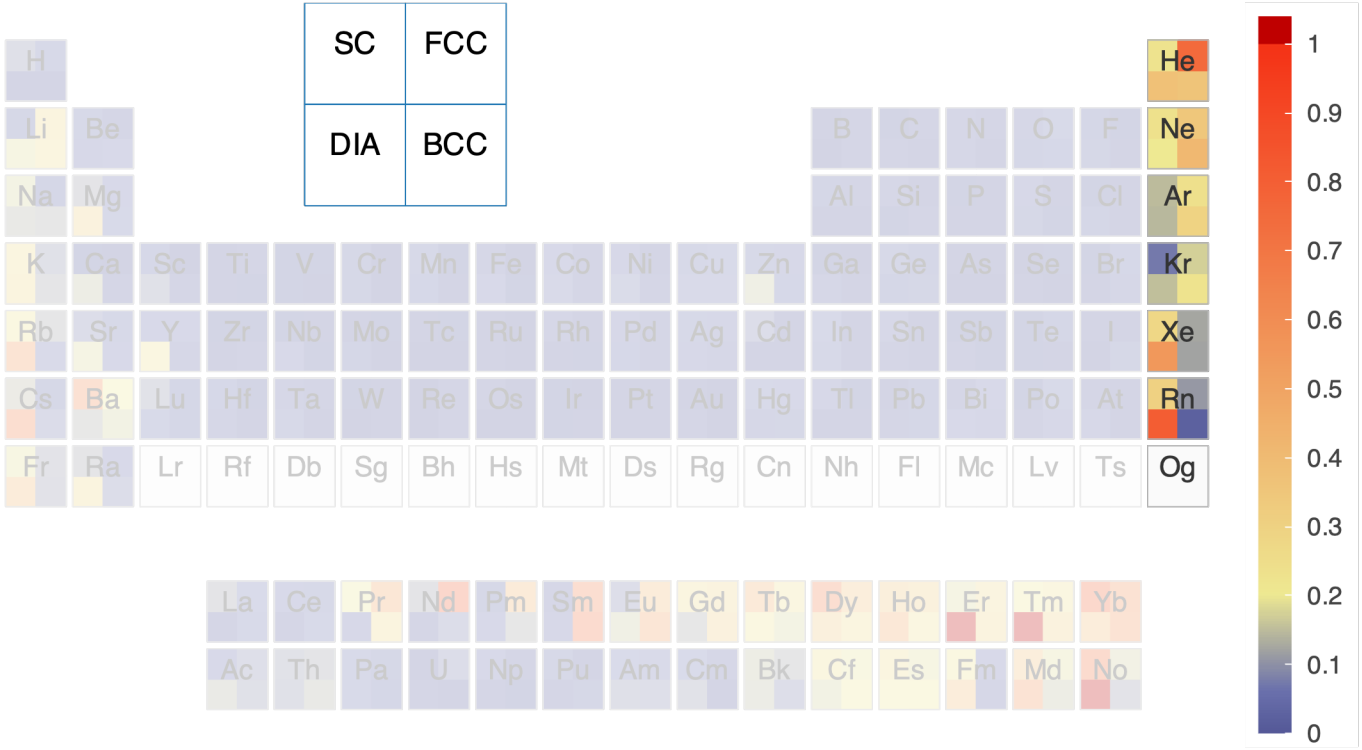
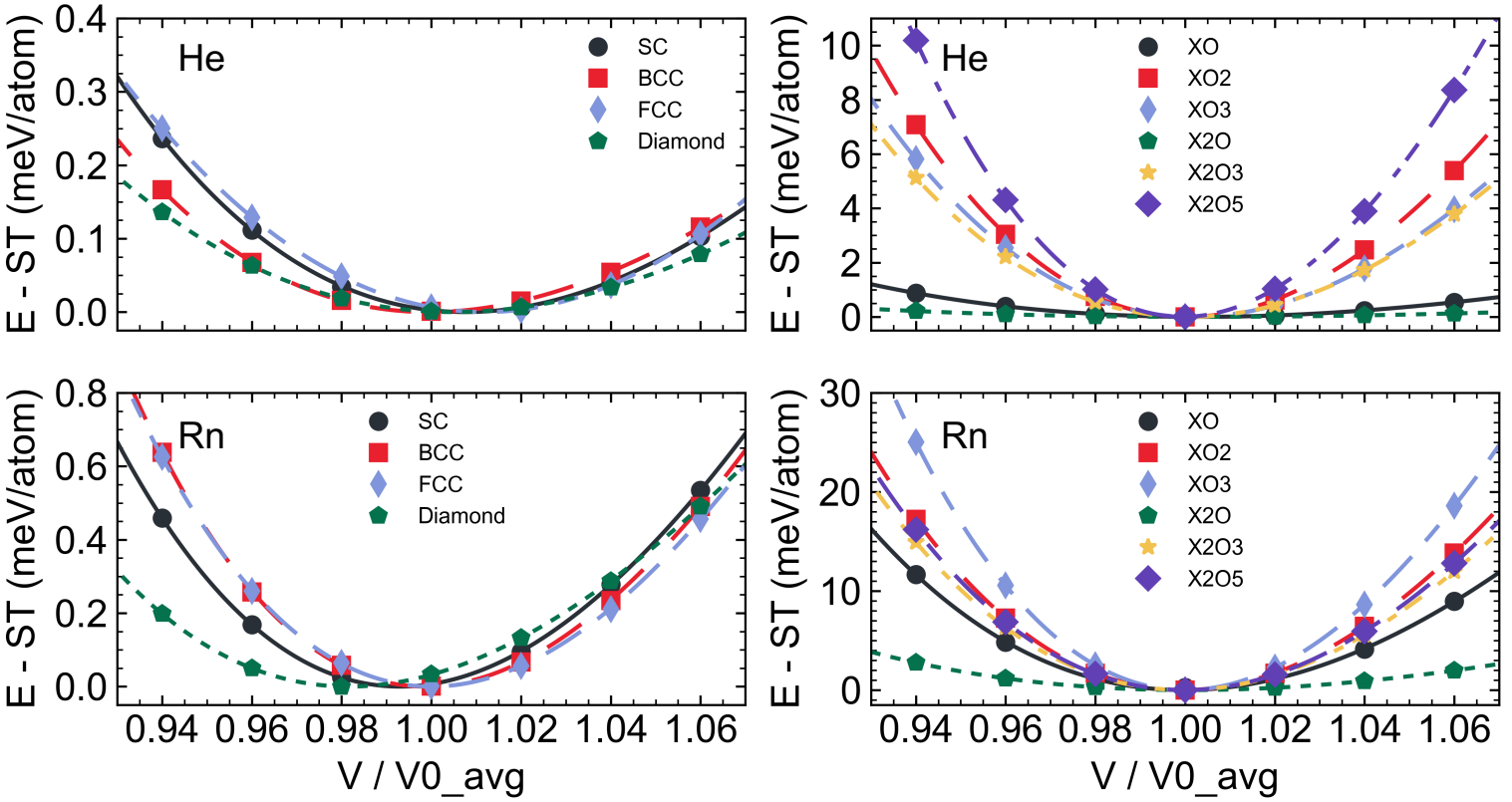
FHI-aims demonstrates good agreement outside a few problem areas



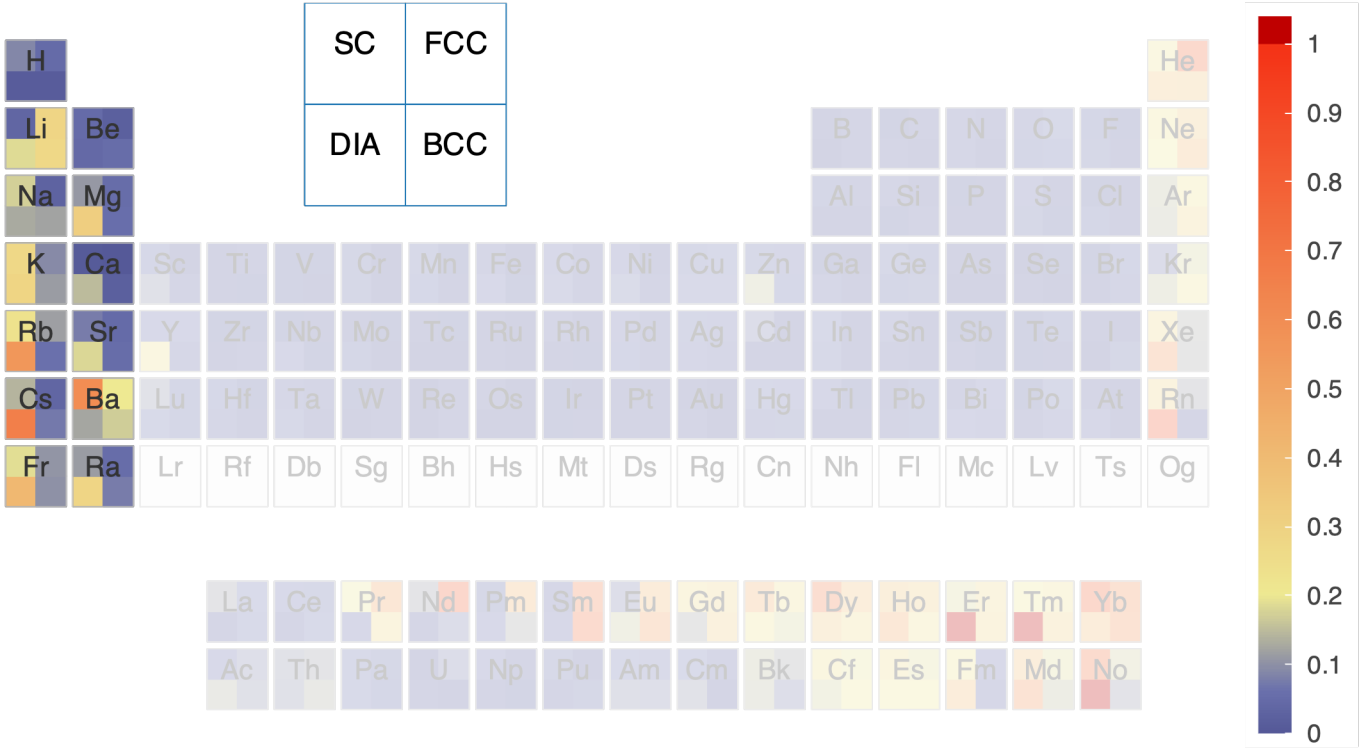
The Noble Gases



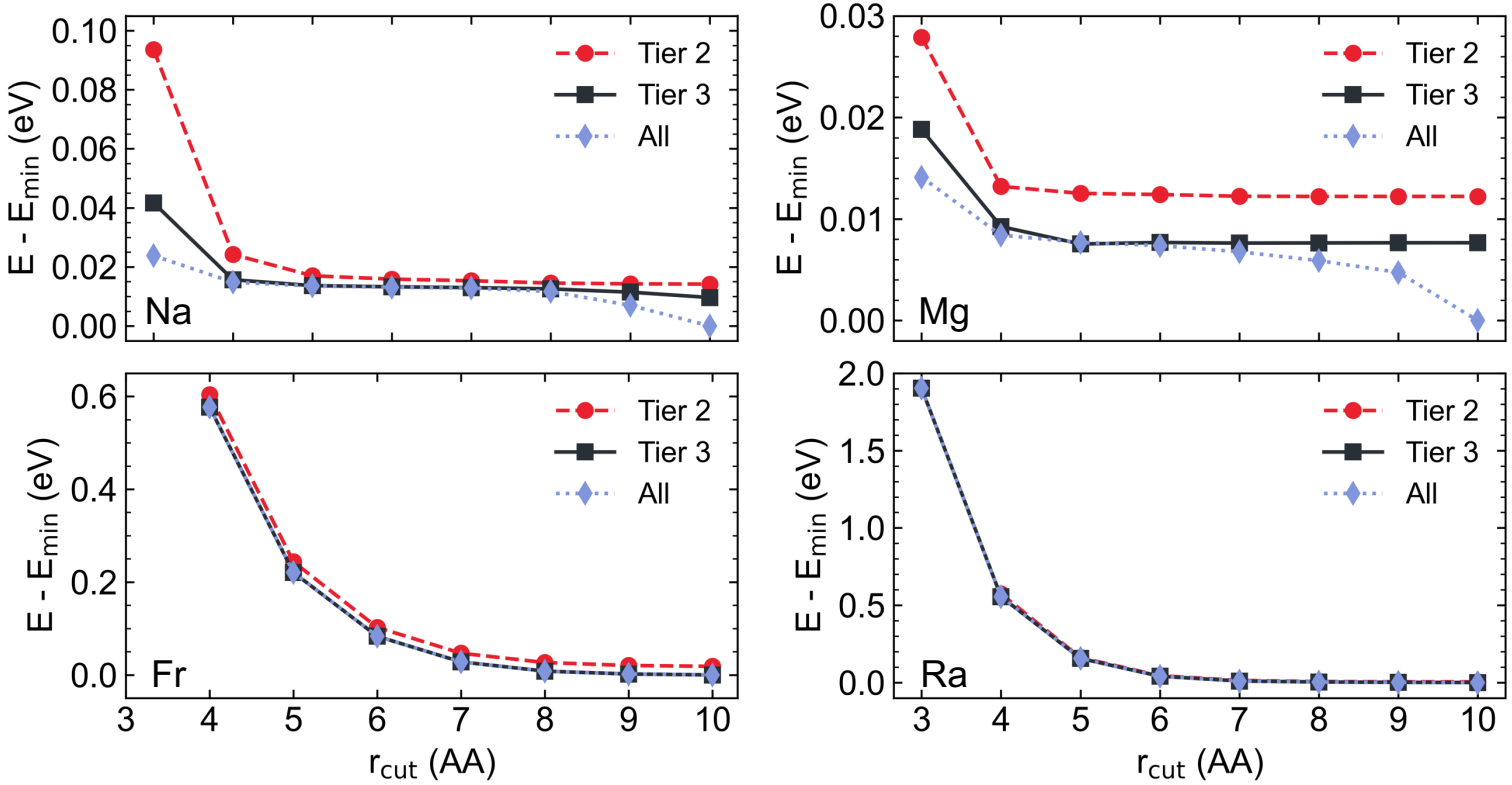
Weak “bonding” potentials increases affect of smaller errors



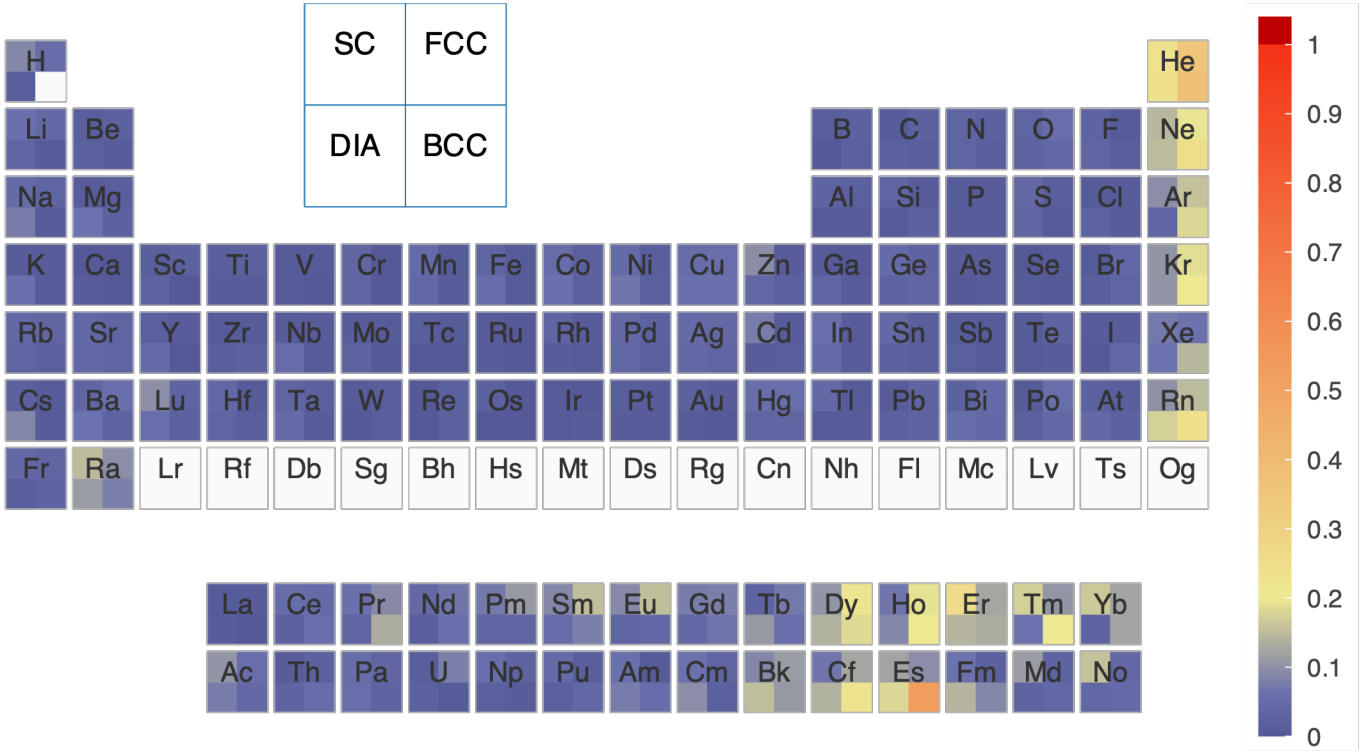
Group 1 and 2 atoms



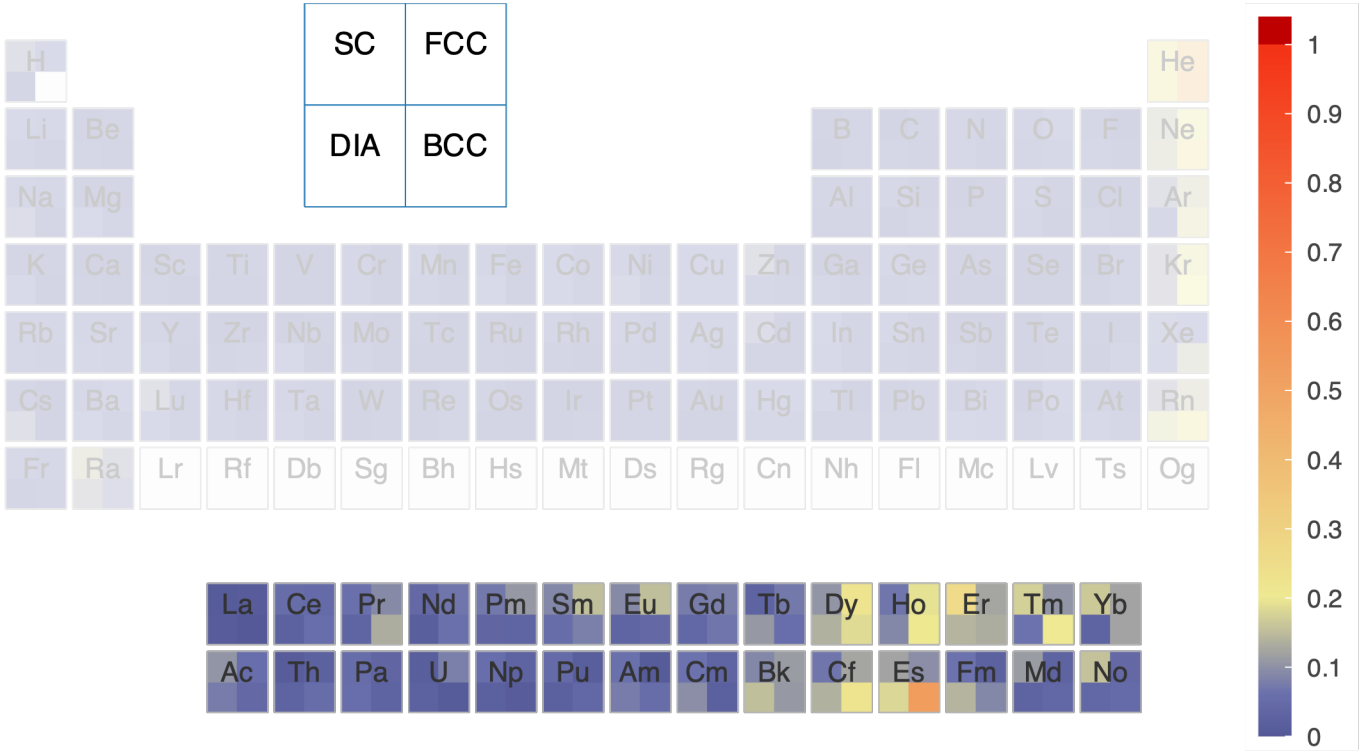
Further refinement of cutoff radii is needed



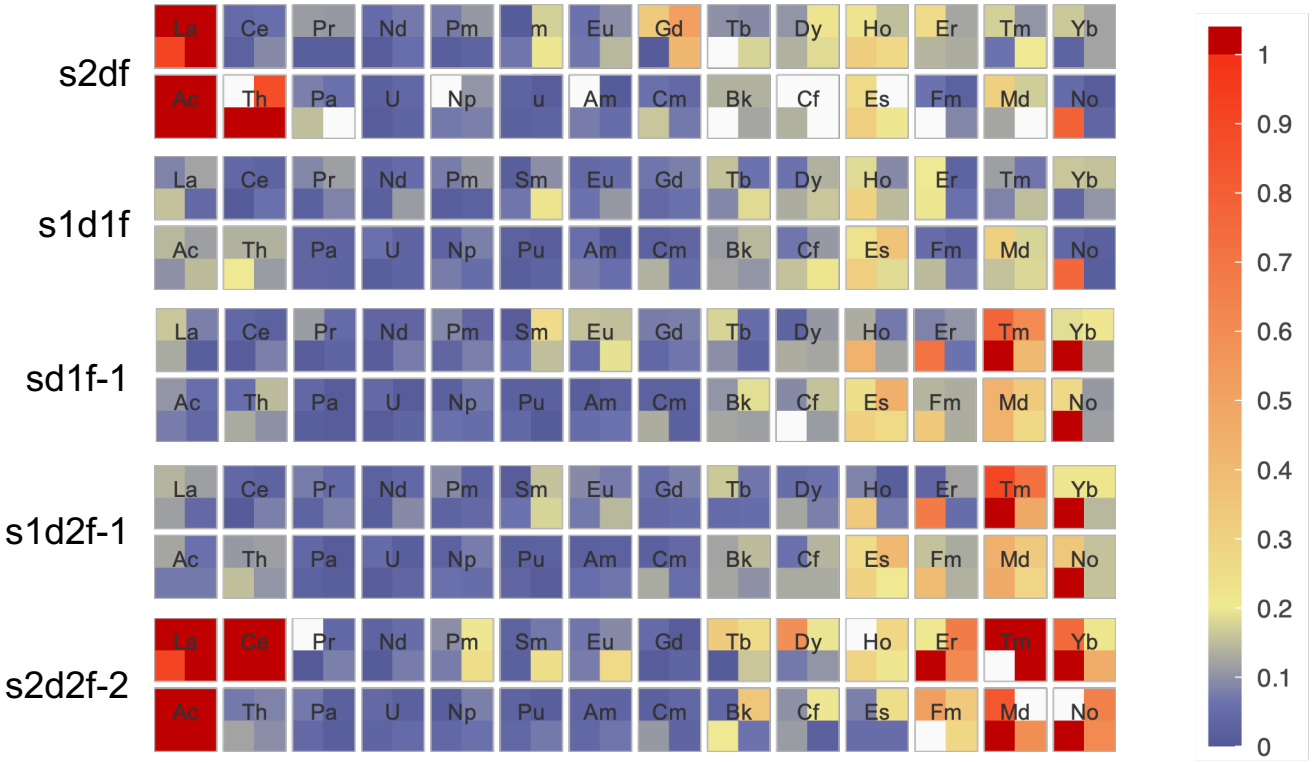
What if we optimize for all standard basis set options?



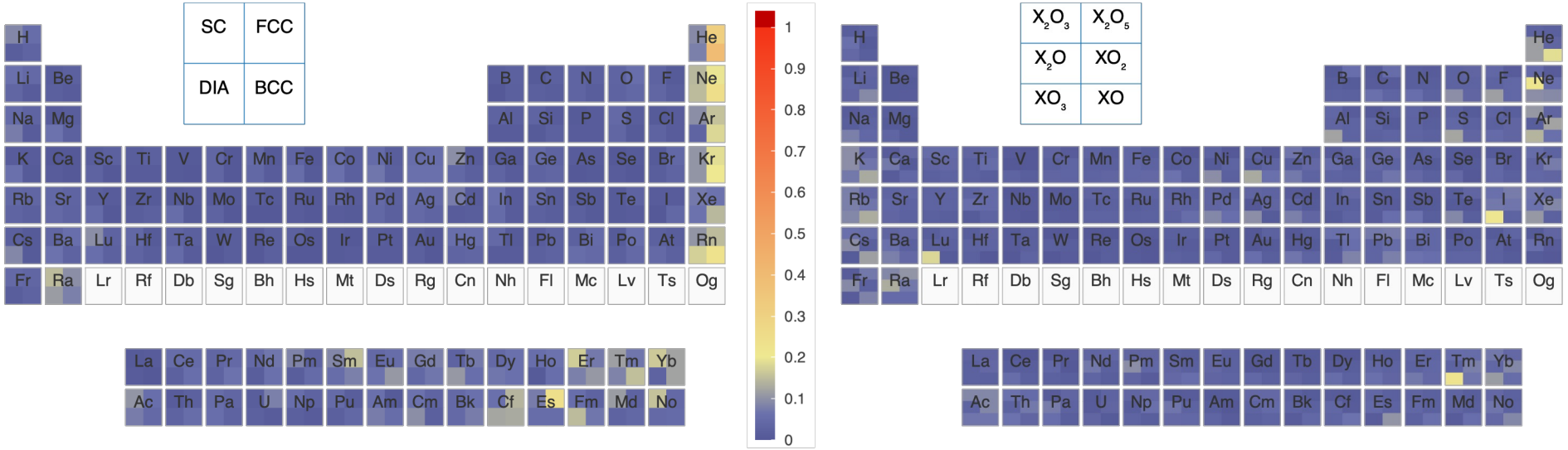
The f-block remains problematic



Initial occupation guesses determine performance



With all improvements FHI-aims consistent with all-electron codes



Discussion Time

Discussion Topics

- ASE
  - What deprecation schedule do we want to have?
  - What is necessary for the interface to do for your external codebases to work?
- pyfhiaims
  - How do we want to maintain it?
  - What should we add to support your calculations?
- pymatgen/atomate2
  - Are there particular workflows we should add?
  - Who uses the interfaces?