Objective #3
Learn how a pure plane wave code functions

How?
Implement a (toy) plane wave code to calculate the band structure of Si

- To plot the band structure of Si (as predicted by Slater exchange)
  - 1). Initial setup (reciprocal-space grid (basis), kinetic energy cutoff, etc.)
  - 2). Converge density
  - 3). Determine eigenvalues at “special” KPs (irreducible BZ)

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How?
Implement a (toy) plane wave code to calculate the band structure of Si

- 1). Initial setup
  - Choice of k-point mesh: Monkhorst-Pack (216 k-points)
  - Kinetic energy cutoff: 150 Ry
  - Si lattice parameter: 10.26 Bohr
  - FCC (real and reciprocal) lattice vectors and atomic positions
  - Pseudopotential (local and/or non-local): Appelbaum-Hamann

$$v(G) = \exp(-G^2/4\alpha)\left(\underbrace{-Z_{ion}\frac{4\pi}{G^2}}_{\text{Long-Range}} + \underbrace{\left(\frac{\pi}{\alpha}\right)^{3/2}\left(v1 + \frac{v2}{\alpha}\left(\frac{3}{2} - \frac{G^2}{4\alpha}\right)\right)}_{\text{Short-Range}}\right)$$

  - Similar to the local component of the GTH pseudopotentials used in PySCF

$$V_{\text{loc}}(g) = -\frac{4\pi Z_{\text{ion}}}{\Omega g^2} e^{-(gr_{\text{loc}})^2/2} + \sqrt{8\pi^3}\frac{r_{\text{loc}}^3}{\Omega} e^{-(gr_{\text{loc}})^2/2} \times \{C_1 + C_2(3 - g^2 r_{\text{loc}}^2) + C_3[15 - 10(gr_{\text{loc}})^2 + (gr_{\text{loc}})^4] + C_4[105 - 105(gr_{\text{loc}})^2 + 21(gr_{\text{loc}})^4 - (gr_{\text{loc}})^6]\}$$

$$\alpha = \frac{1}{2r_{loc}^2}$$

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How?
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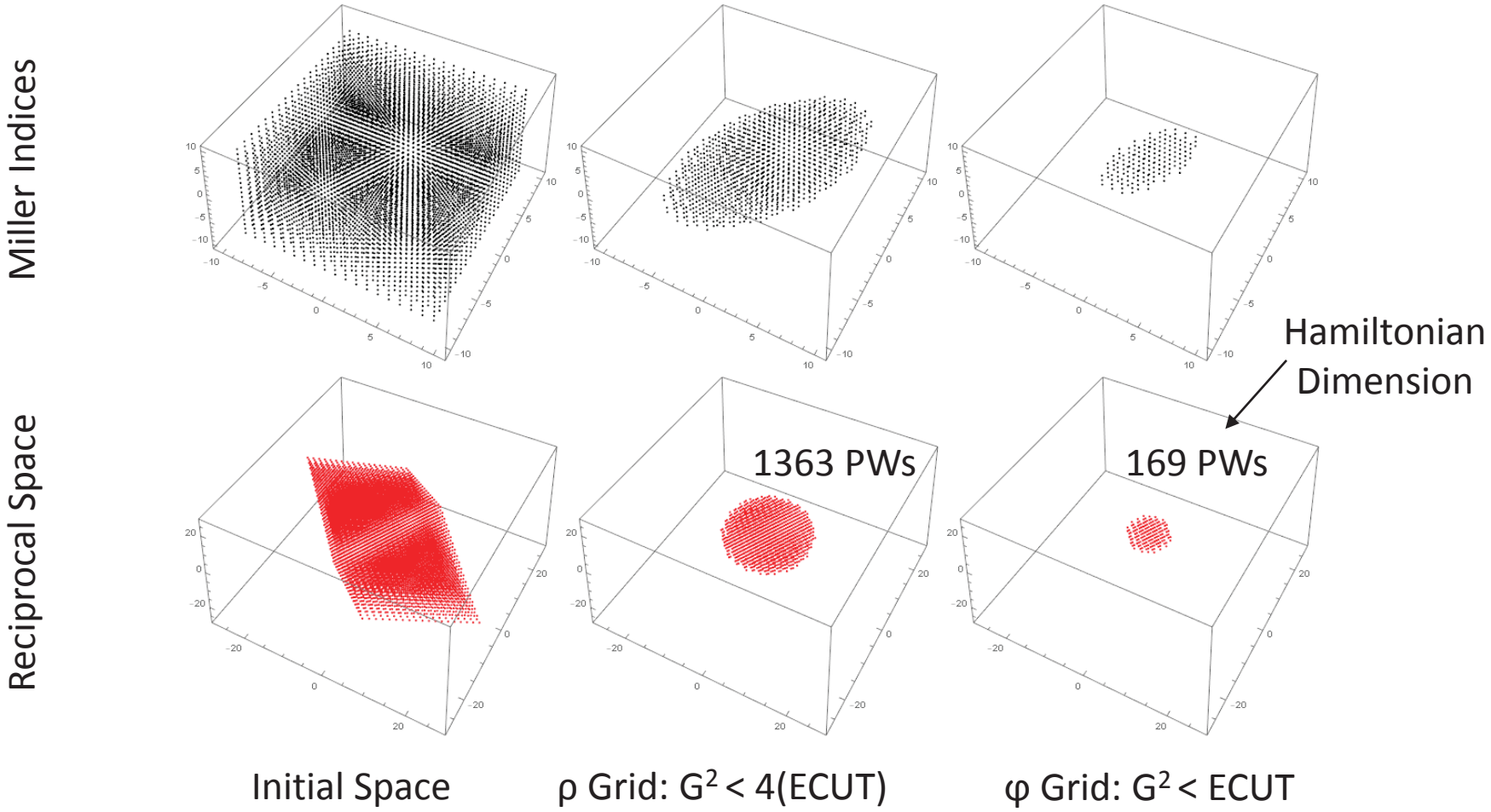
- 1). Initial setup
  - Reciprocal-space grid (determined by kinetic energy cutoff, ECUT)



  - # of plane waves for density ≈ 8 x (# of plane waves for orbitals)

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- 2). Converge density
  - For all k-points:
    - Form Hamiltonian
      - Diagonal elements get kinetic energy contribution, $\propto (\mathbf{k} + \mathbf{G})^2$
      - All elements get potential (pseudo x structure factor + Coulomb + Vxc)
    - Diagonalize Hamiltonian
      - This gives eigenvalues (for plotting band structure) as well as eigenvectors for evaluating the density
    - Accumulate density (over all k-points) by summing over occupied bands
  - Check convergence of density
  - Evaluate Vxc (on real space grid, then FFT to reciprocal space)
  - Evaluate Coulomb (in reciprocal space, after IFFT of density to reciprocal space)
    - $4\pi\rho(G)/G^2$
  - Iterate until convergence

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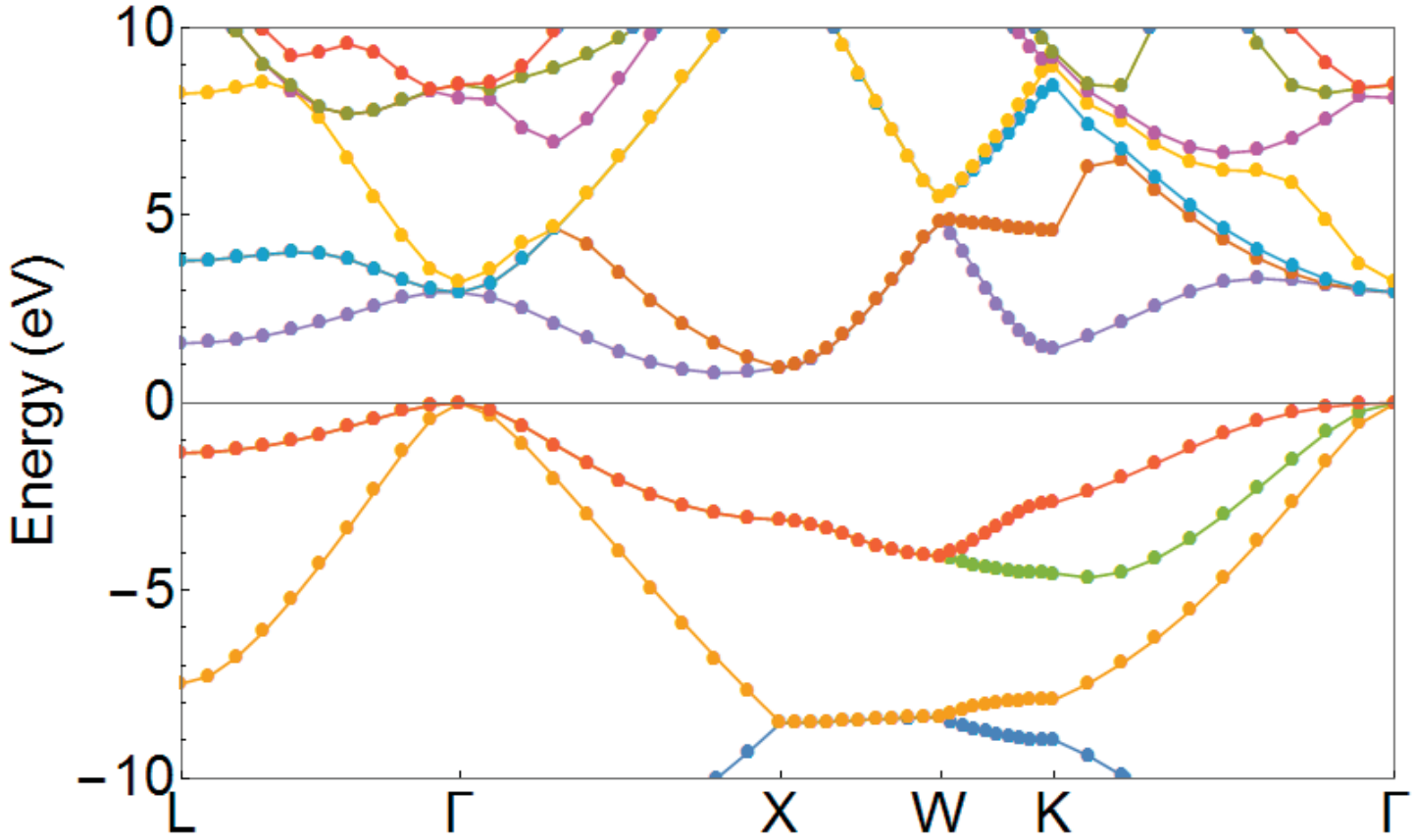
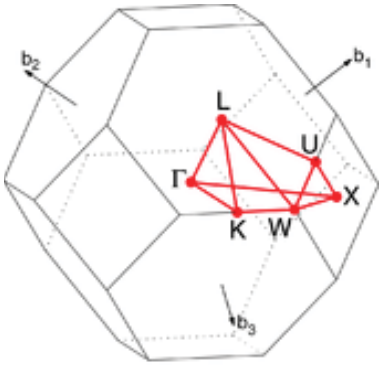
- 3). Determine eigenvalues at “special” KPs (non-self-consistently)
  - Set up a new k-point mesh (over N special points)
  - Form Hamiltonian (using converged density) and diagonalize N times



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The indirect band gap is 0.795 ev
The direct band gap is 2.94 ev
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