Green's function approach to *ab initio* band structures

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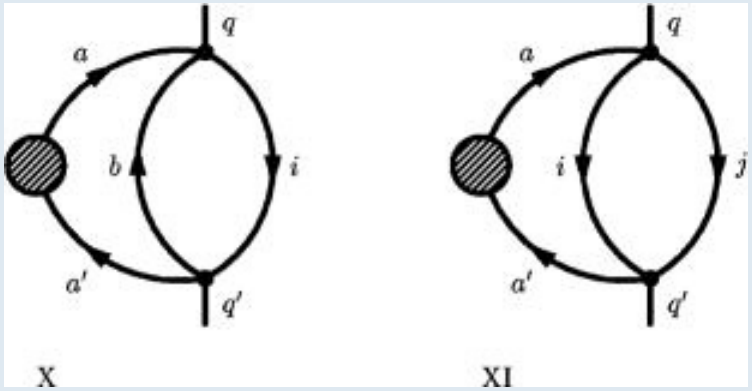
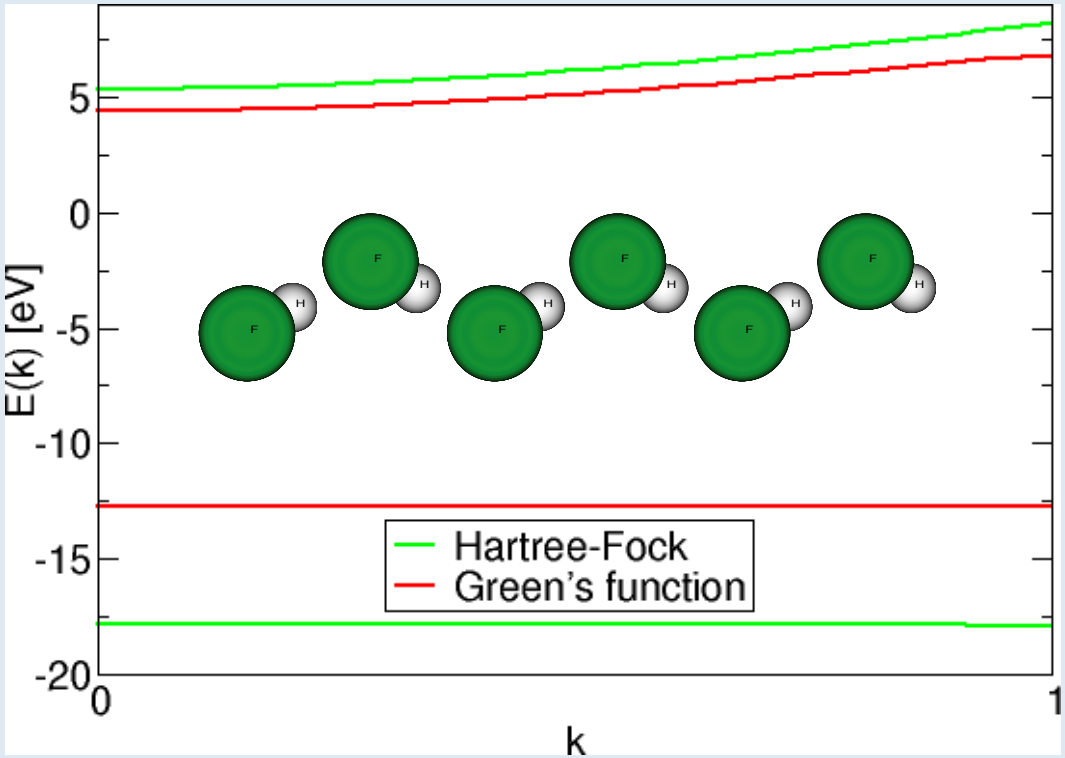


First principles methods

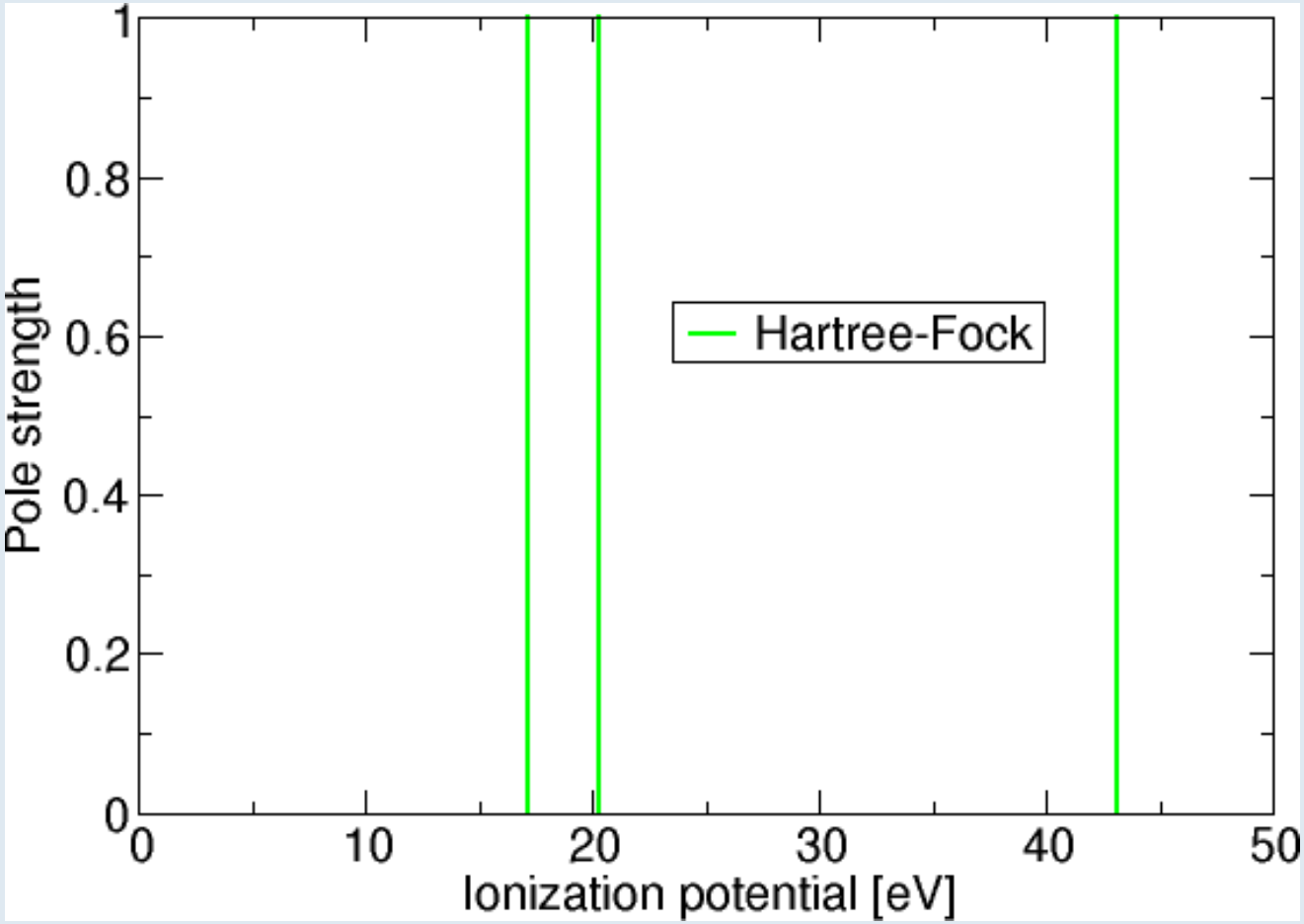
- Schrödinger equation with electronic Hamiltonian
- Independent particle/quasi-particle theories
  - *Ab initio* (wavefunction based): Hartree-Fock
  - Density functional theory
- **But** there are many-body effects beyond the quasi-particle picture

Band structures

- Energy levels of crystals
- Resolved with respect to translational symmetry
- Example: hydrogen fluoride polymer



Strong correlation: a single hydrogen fluoride molecule



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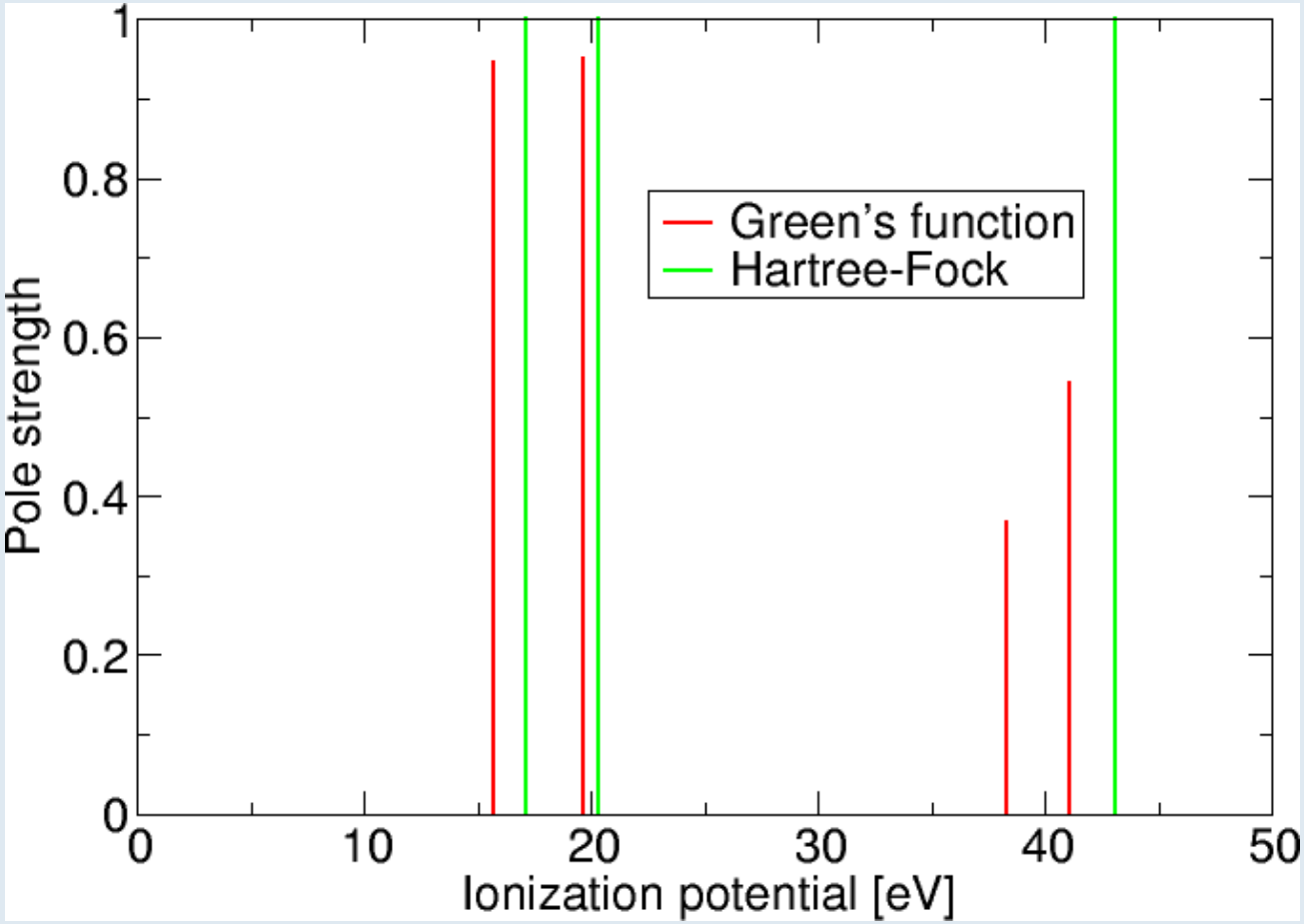

Crystal orbital algebraic diagrammatic construction

- CO-ADC was derived from the molecular equations (part of my thesis)
- Based on Wannier orbitals
- Band structures are calculated in terms of an eigenvalue problem

$$\mathbf{B}(\vec{k}) = \begin{pmatrix} \boldsymbol{\varepsilon}(\vec{k}) + \boldsymbol{\Sigma}^{\infty}(\vec{k}) & \mathbf{U}_{\mathrm{I}}^{+} & \mathbf{U}_{\mathrm{II}}^{+} \\ \mathbf{U}_{\mathrm{I}}(\vec{k}) & \mathbf{K}_{\mathrm{I}} + \mathbf{C}_{\mathrm{I}} & \mathbf{0} \\ \mathbf{U}_{\mathrm{II}}(\vec{k}) & \mathbf{0} & \mathbf{K}_{\mathrm{II}} + \mathbf{C}_{\mathrm{II}} \end{pmatrix}$$

Conclusion

- *Ab initio* methods facilitate to predict properties of solids
- Electron correlation plays a significant role for band structures

- Strong correlation can be examined with advanced Green‘s function methods
- CO-ADC will be applied in the near future