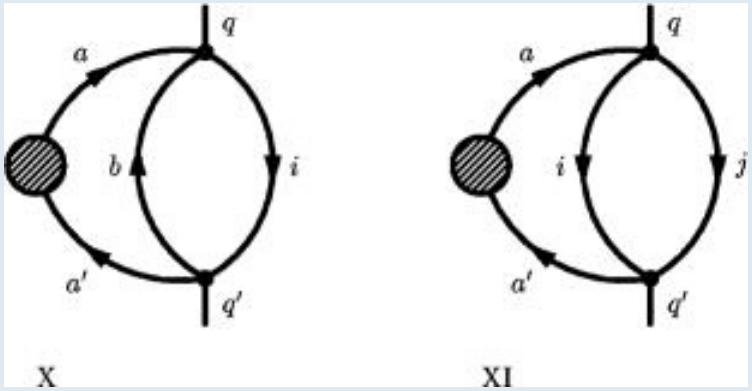
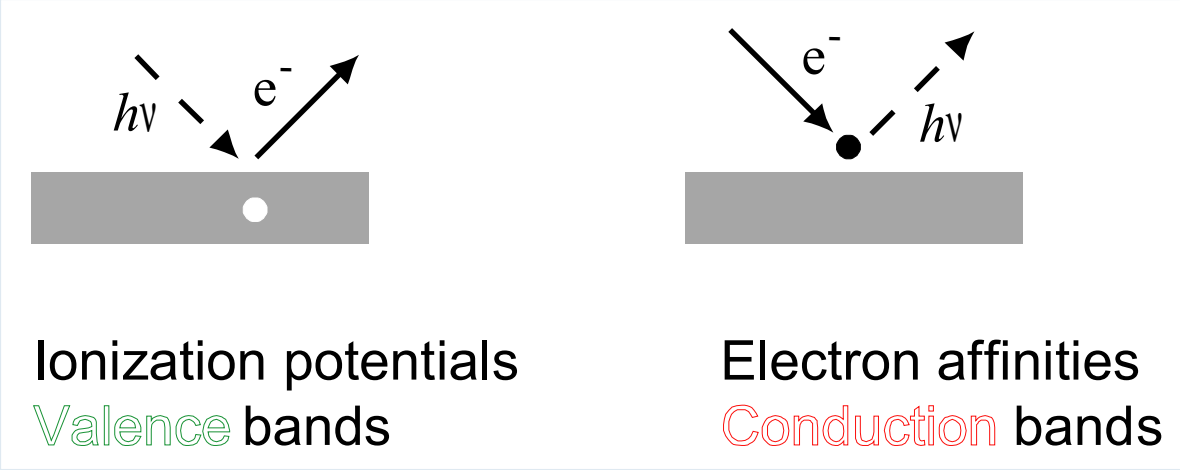
Green's function approach to *ab initio* band structures

Christian Buth



First principles!

- Excited states of solids



- Full Hamiltonian
- Start: Hartree-Fock approximation

Crystal orbital algebraic diagrammatic construction

- Many-body Green's functions
  - Dyson equation
  - Crystal orbital algebraic diagrammatic construction (CO-ADC)
- Hermitian eigenvalue problem

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

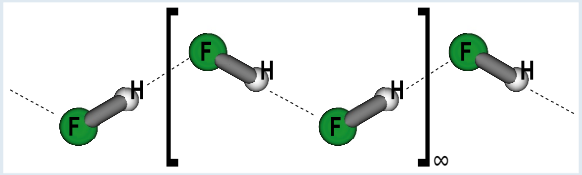
Correlated band structures

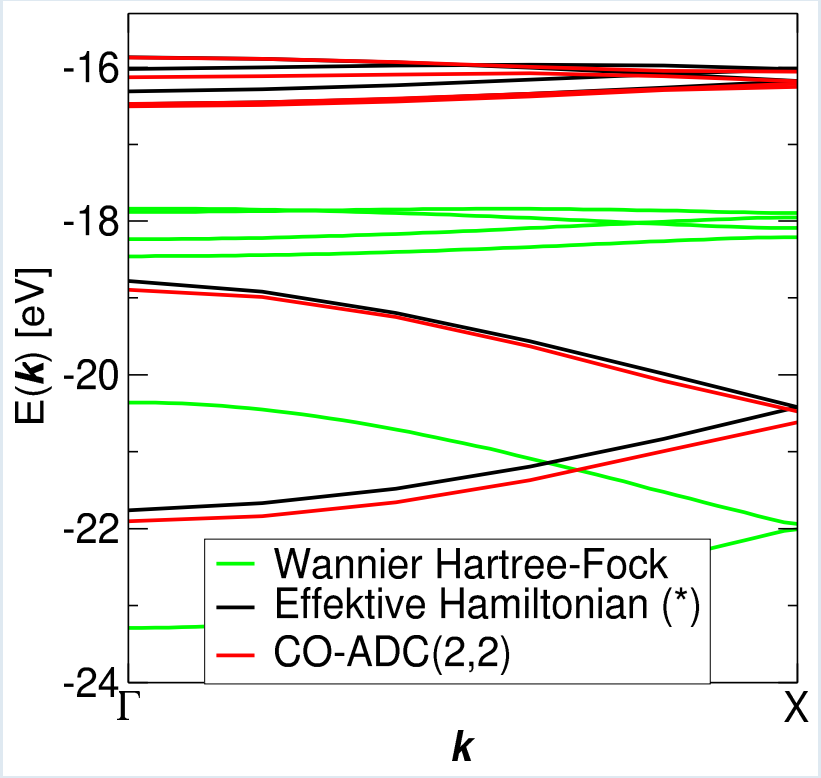
- *Ab initio* approach
- Spectral method
  - Strong correlation
  - Electronic resonances
- Computer program was developed

[Theory: Buth, Birkenheuer, Albrecht, Fulde: arXiv:cond-mat/0409078]

Hydrogen fluoride chain

- Energy levels of crystals
- Translational symmetry classified

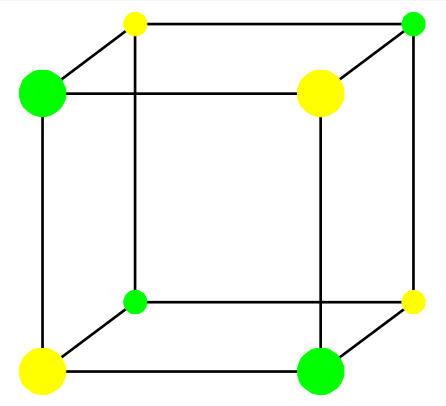


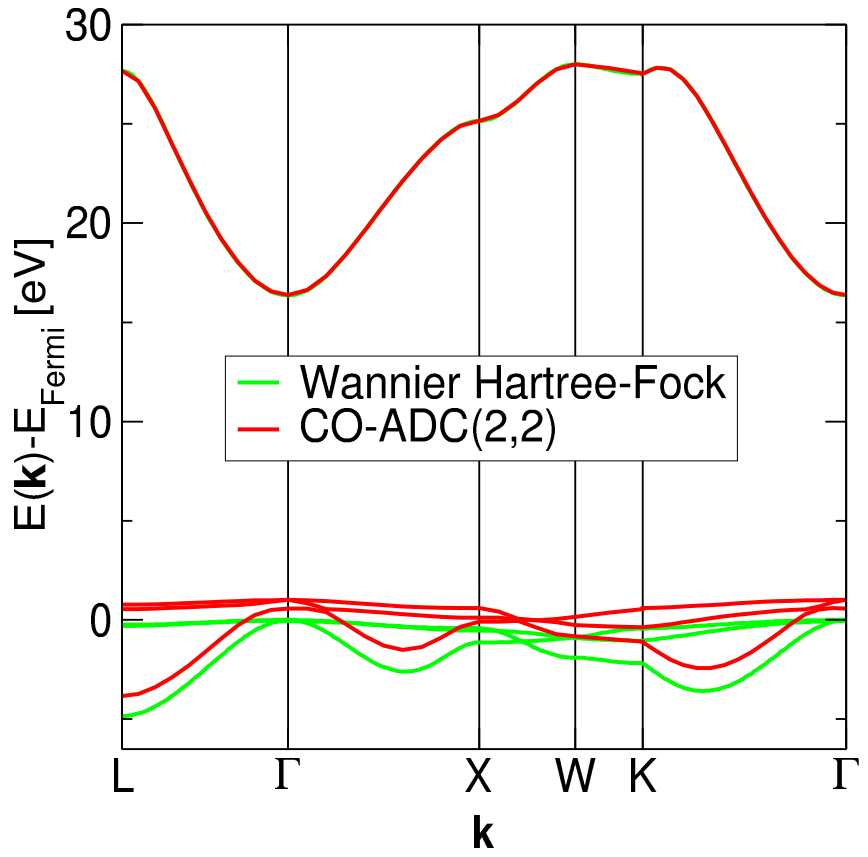


(*) Calculation by **Viktor Bezugly**
[Theory: Bezugly, Birkenheuer: Chem. Phys. Lett. **399** 57 (2004)]

Lithium fluoride crystal

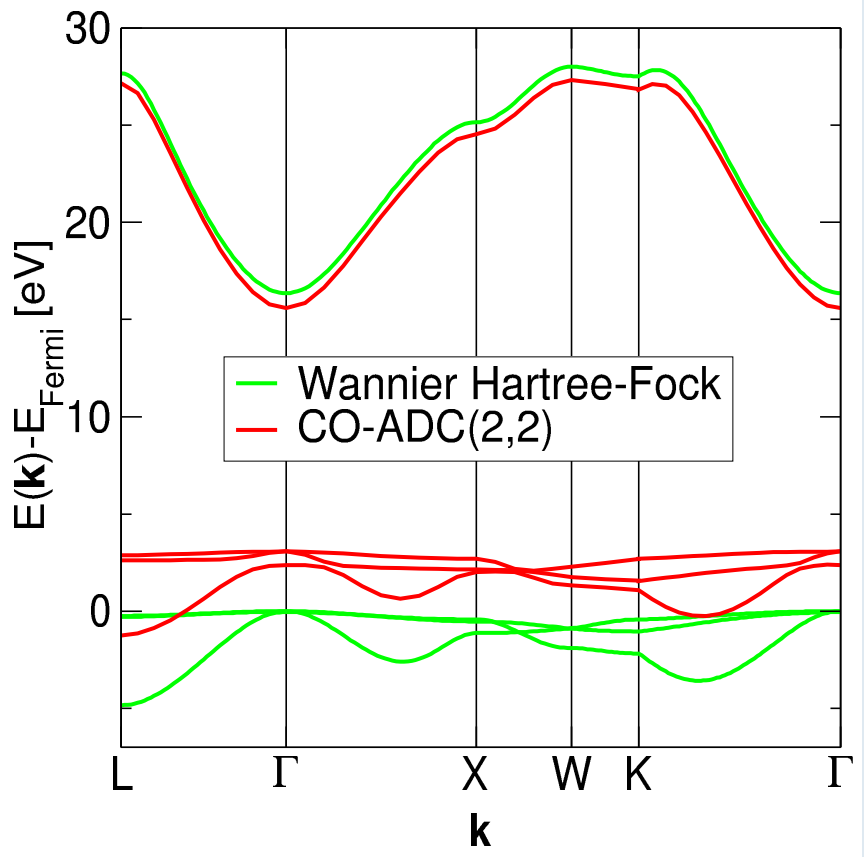
- Excitations from origin cell
- Upwards shift of valence bands
- Conduction band unchanged



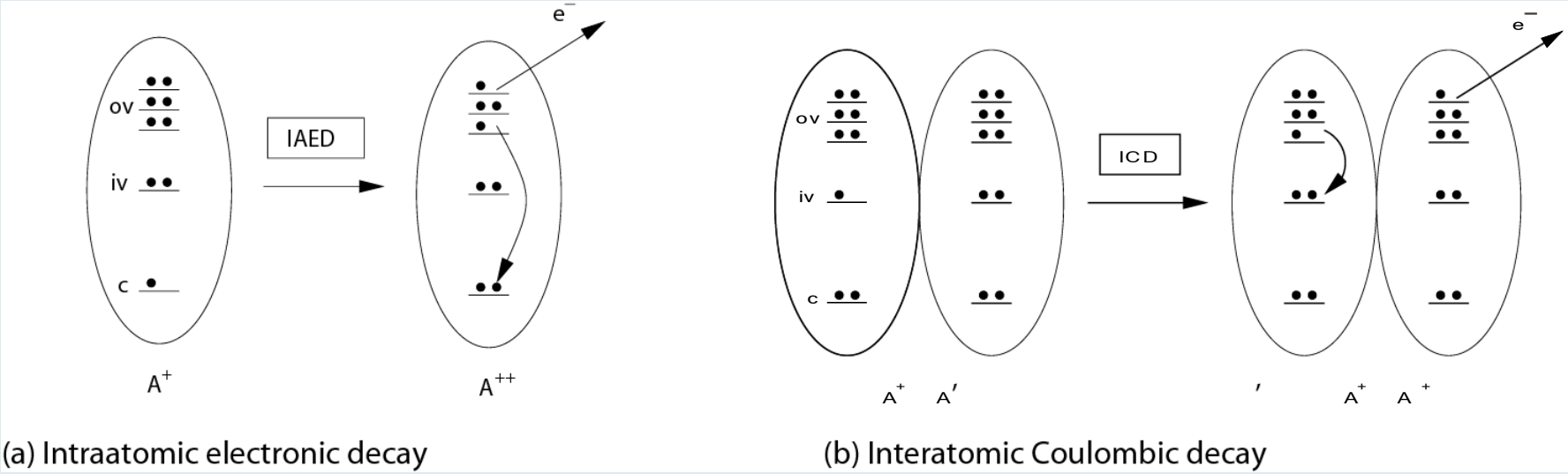


Lithium fluoride crystal

- Excitations from 19 unit cells
- Shift of bands increased
- Good agreement with experiments



Auger decay



(a) Intraatomic electronic decay

(b) Interatomic Coulombic decay

- Intra- and interatomic contributions, ultra fast
- Deep insight into many-body effects
- Presently intense experimental studies

[Buth, Santra, Cederbaum, J. Chem. Phys. **119** 10575 (2003)]

Conclusion

- Electron correlations are important
- CO-ADC is a powerful *ab initio* method for band structures
  - Hermitian eigenvalue problem
  - Strong correlation
  - Intra- and interatomic effects
  - Electronic resonances (Auger decay)
- Merry Christmas!