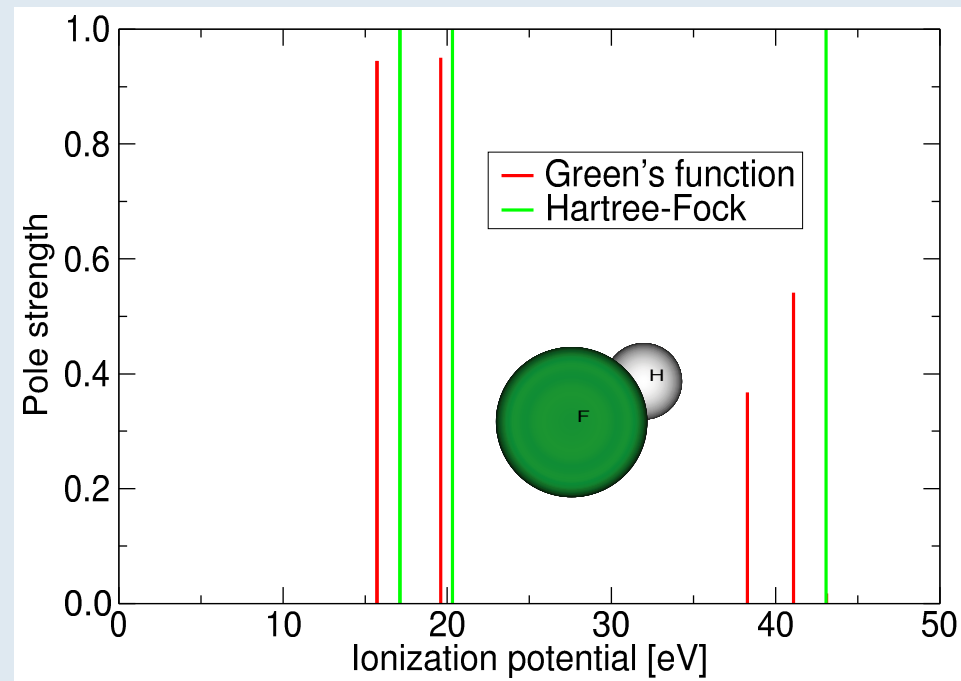


Green's function approach to *ab initio* band structures

Christian Buth

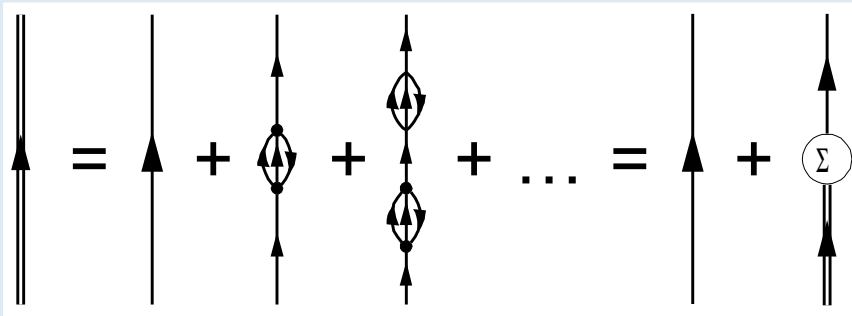
Max-Planck-Institut für Physik komplexer Systeme, Dresden, Germany

- There are many-body effects beyond the quasi-particle picture!



Crystal orbital ADC

- One-particle Green's function
- Dyson equation



- *Intermediate* representation of $\Sigma(\vec{k}, \omega)$ in terms of Wannier orbitals
- Band structure from a Hermitian *eigenvalue problem*
- Configuration selection

Correlated band structures

- Band structure of
 - HF chains
 - LiF crystals
- Assessment of the perturbative treatment of the off-diagonal Fock matrix elements within CO-ADC

