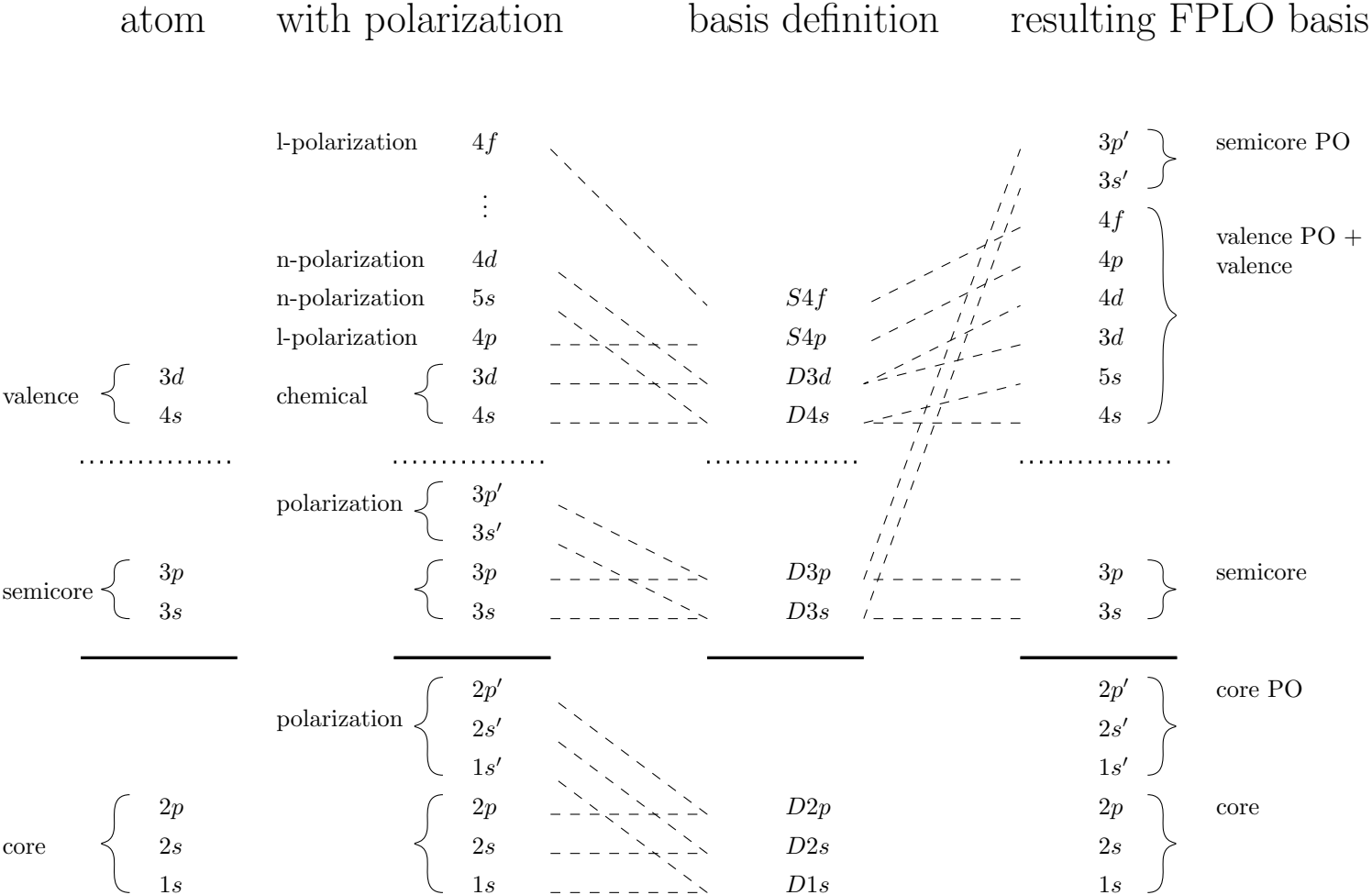
atom
with polarization
basis definition
resulting FPLO basis
l-polarization
4f
n-polarization
4d
n-polarization
5s
l-polarization
4p
valence
3d
4s
chemical
3d
4s
S4f
S4p
D3d
D4s
3p′
3s′
4f
4p
4d
3d
5s
4s
semicore PO
valence PO +
valence
polarization
3p′
3s′
semicore
3p
3s
D3p
D3s
3p
3s
semicore
polarization
2p′
2s′
1s′
core PO
core
2p
2s
1s
D2p
D2s
D1s
2p
2s
1s
core