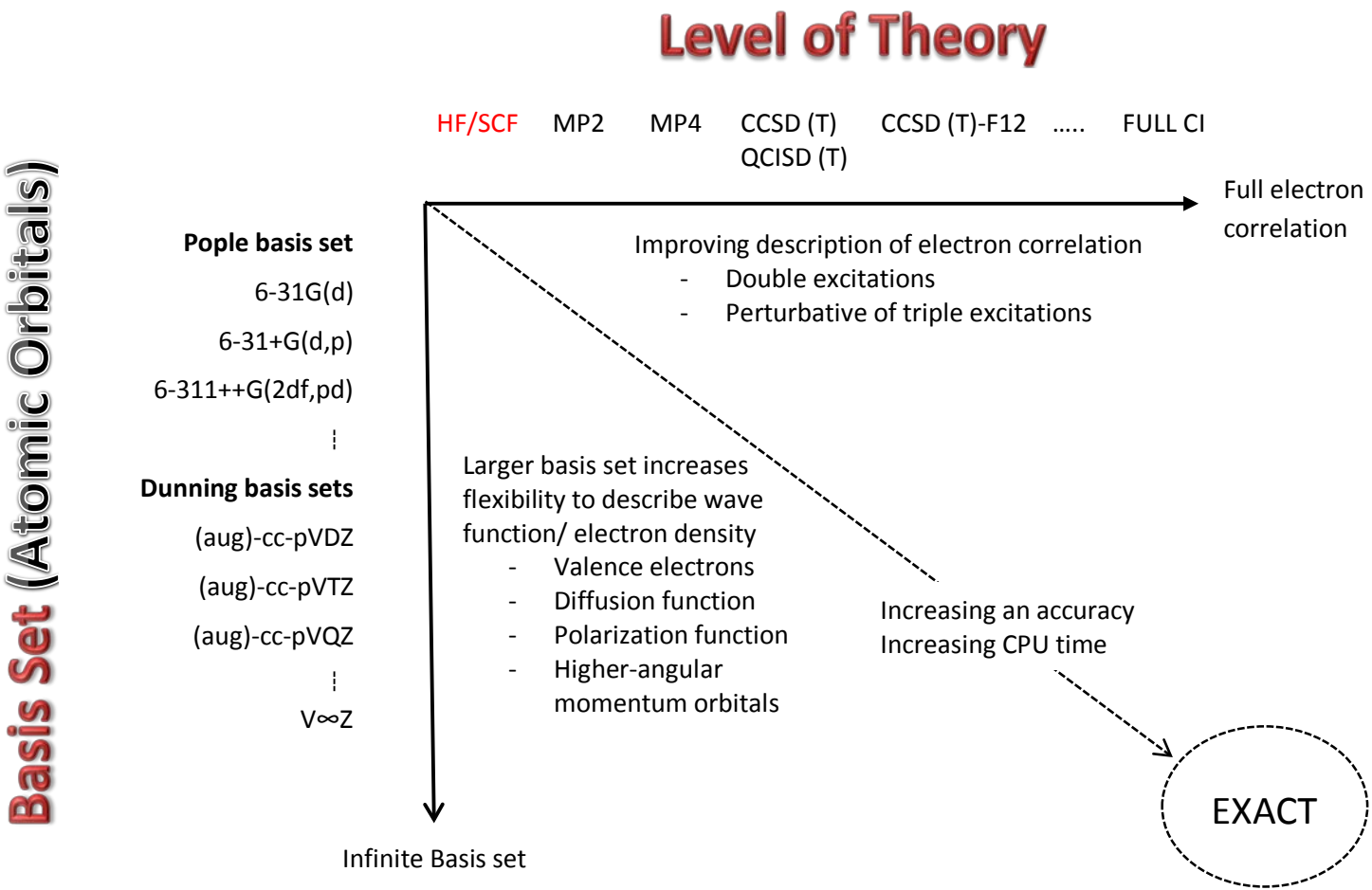
Level of Theory
HF/SCF
MP2
MP4
CCSD (T)
QCISD (T)
CCSD (T)-F12
.....
FULL CI
Full electron correlation
Basis Set (Atomic Orbitals)
Pople basis set
6-31G(d)
6-31+G(d,p)
6-311++G(2df,pd)
Dunning basis sets
(aug)-cc-pVDZ
(aug)-cc-pVTZ
(aug)-cc-pVQZ
V∞Z
Improving description of electron correlation
- Double excitations
- Perturbative of triple excitations
Larger basis set increases flexibility to describe wave function/ electron density
- Valence electrons
- Diffusion function
- Polarization function
- Higher-angular momentum orbitals
Increasing an accuracy
Increasing CPU time
EXACT
Infinite Basis set