

**Initial structure**

**Struct. optimization: DFT+ $U$ + $V$**

**SCF ground state: DFT+ $U$ + $V$**

**Calculation of  $U$  &  $V$ : DFPT**

**$U$  &  $V$  & structure  
converged?**

**No**

**Yes**

**Self-consistent parameters:**

**$U_{\text{scf}}$  &  $V_{\text{scf}}$**

