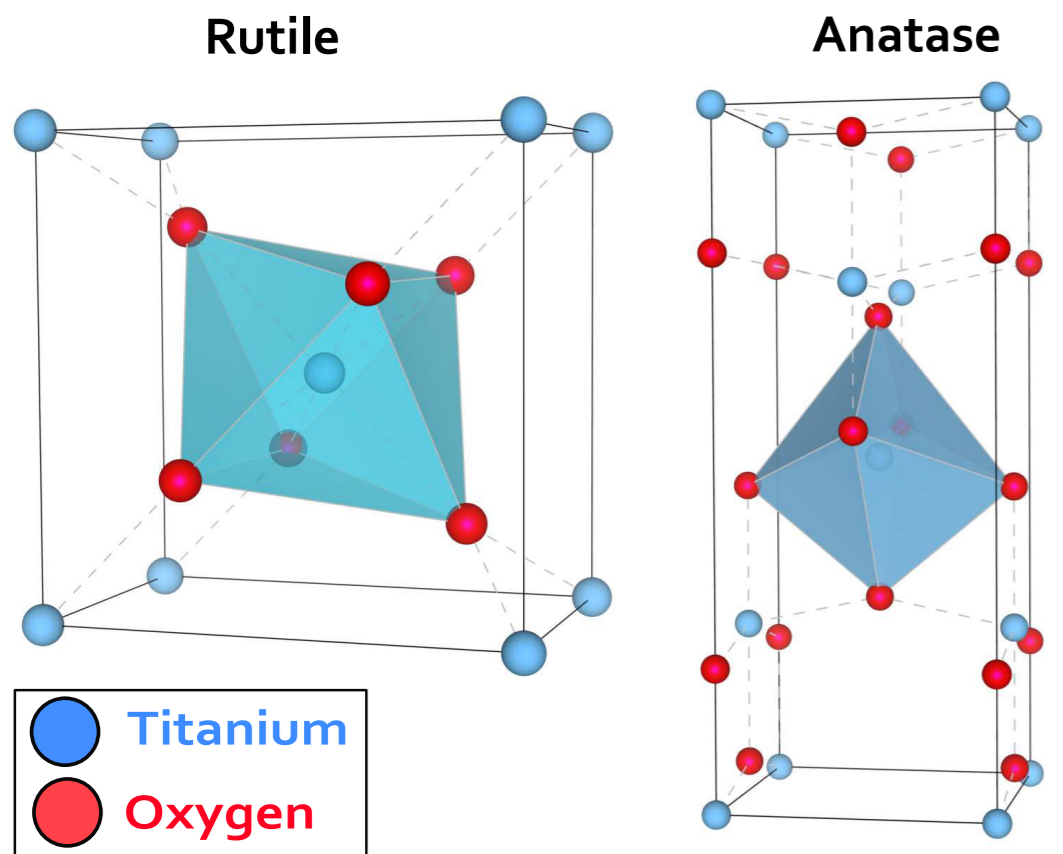
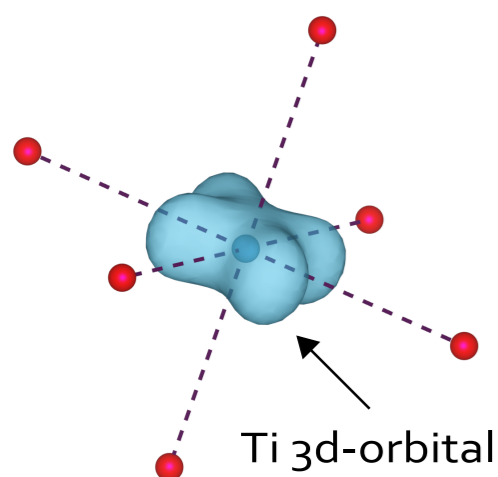


Charge Trapping in Bulk TiO₂ Rutile and Anatase

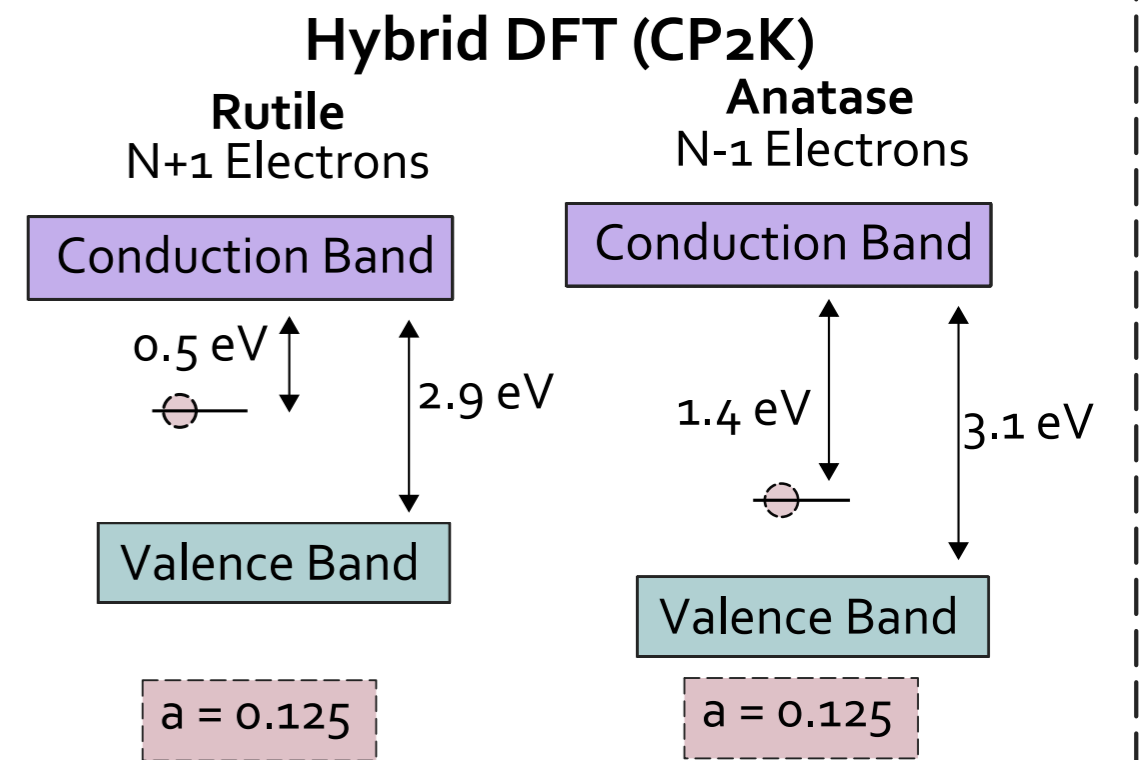
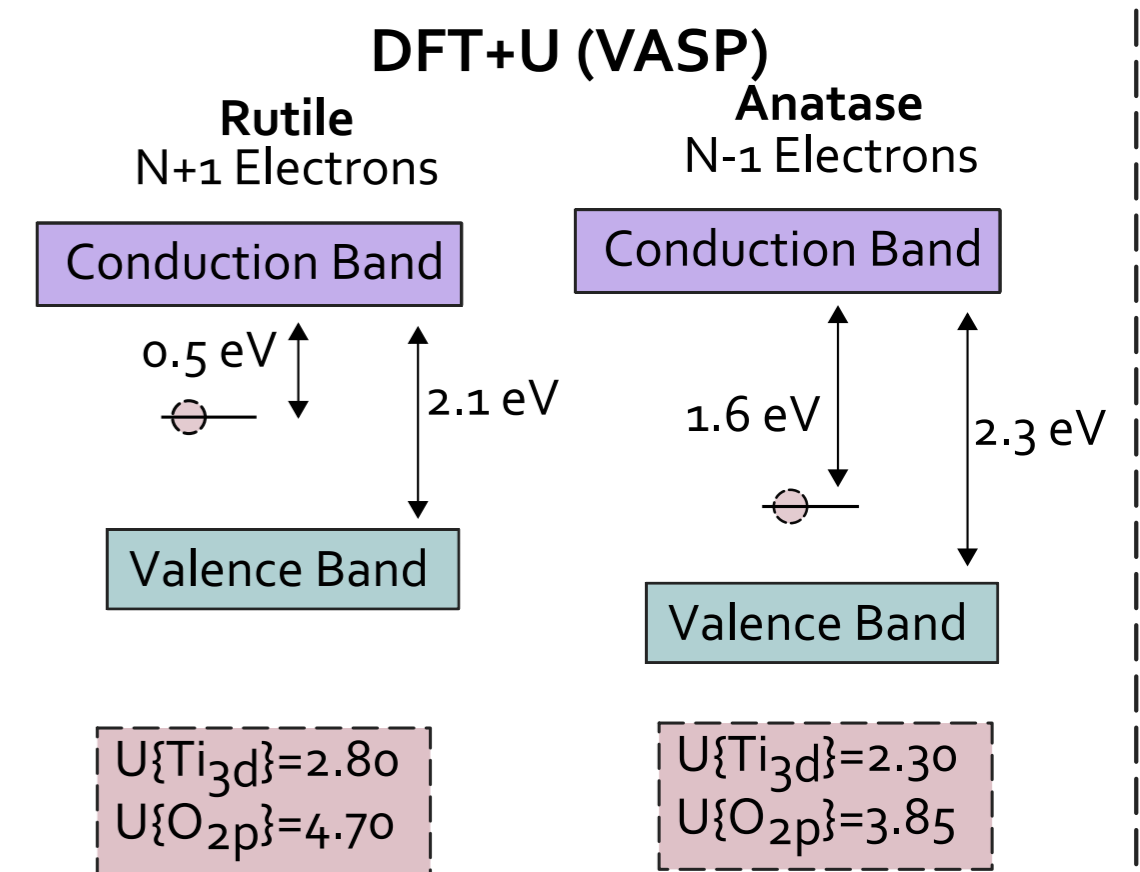
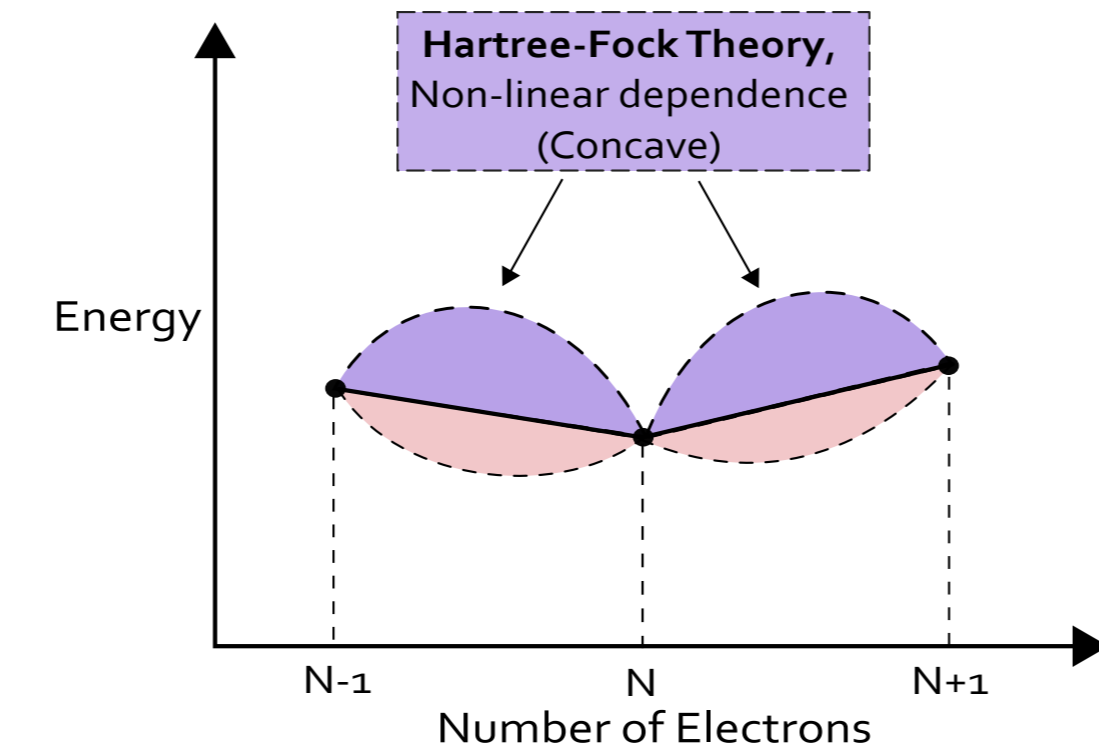
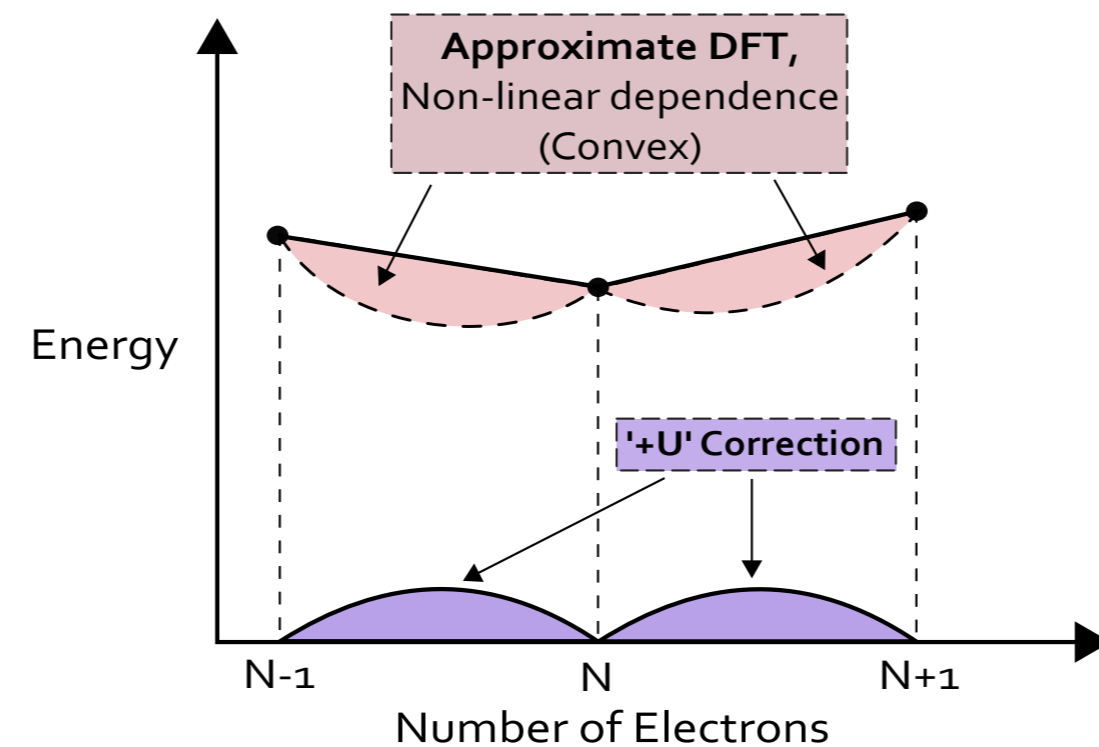
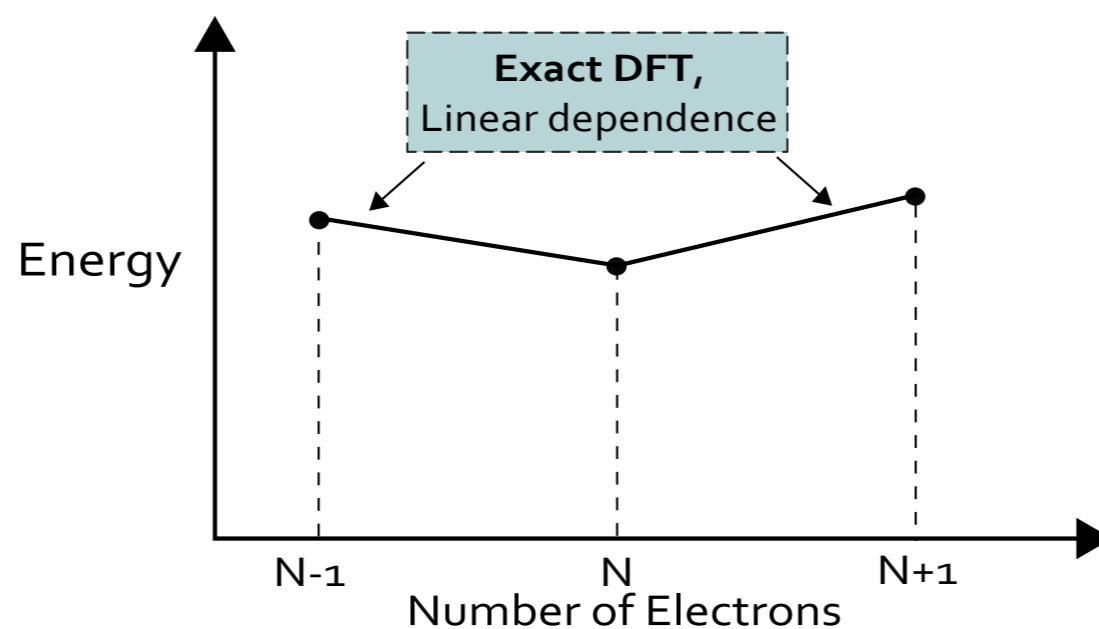
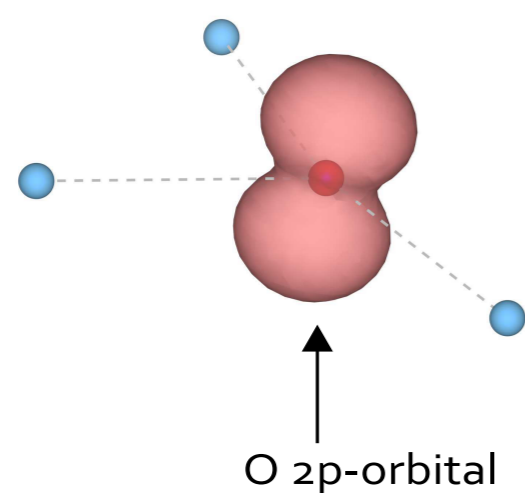
Me: Razak Elmaslmane
Supervisor: Keith McKenna
University of York



Rutile:
Electron polaron



Anatase:
Hole polaron



Finite size effects not (yet) considered for hybrid DFT results

Bulk TiO₂ Modifications

DFT+U → Non-linearity changes dramatically

Hybrid DFT → Non-linearity changes very little