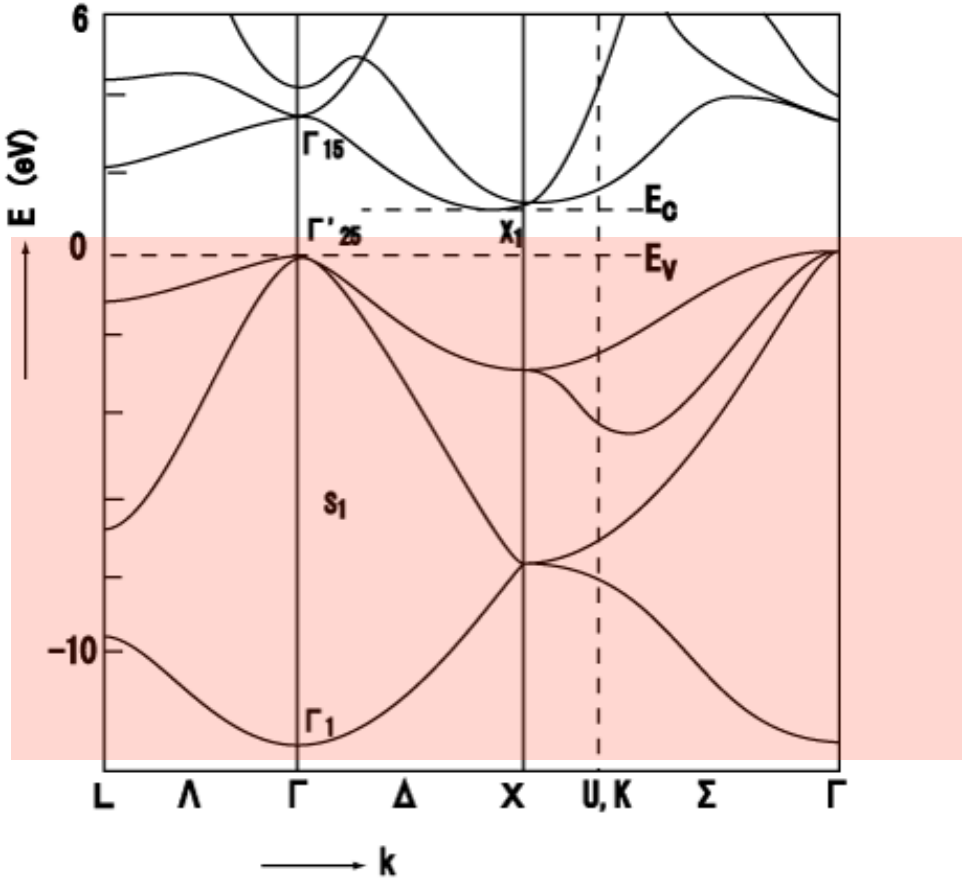
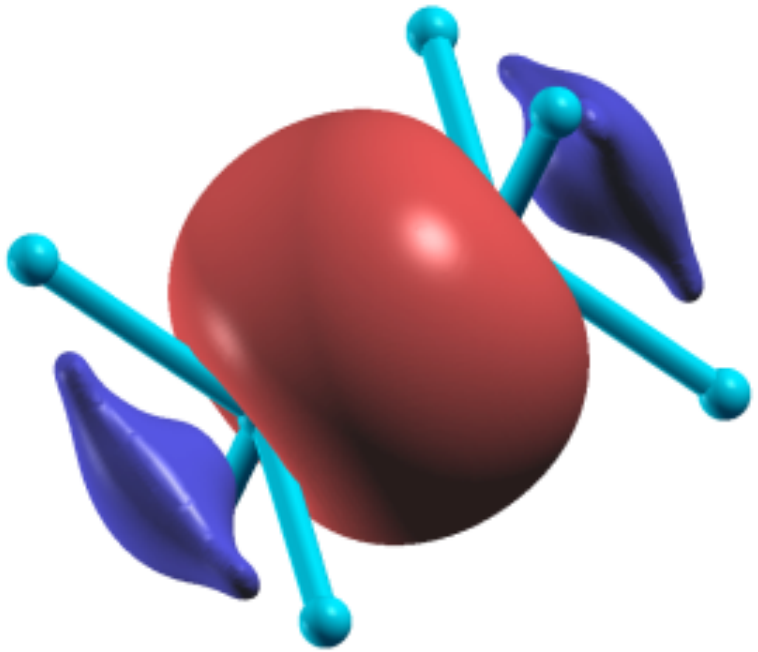
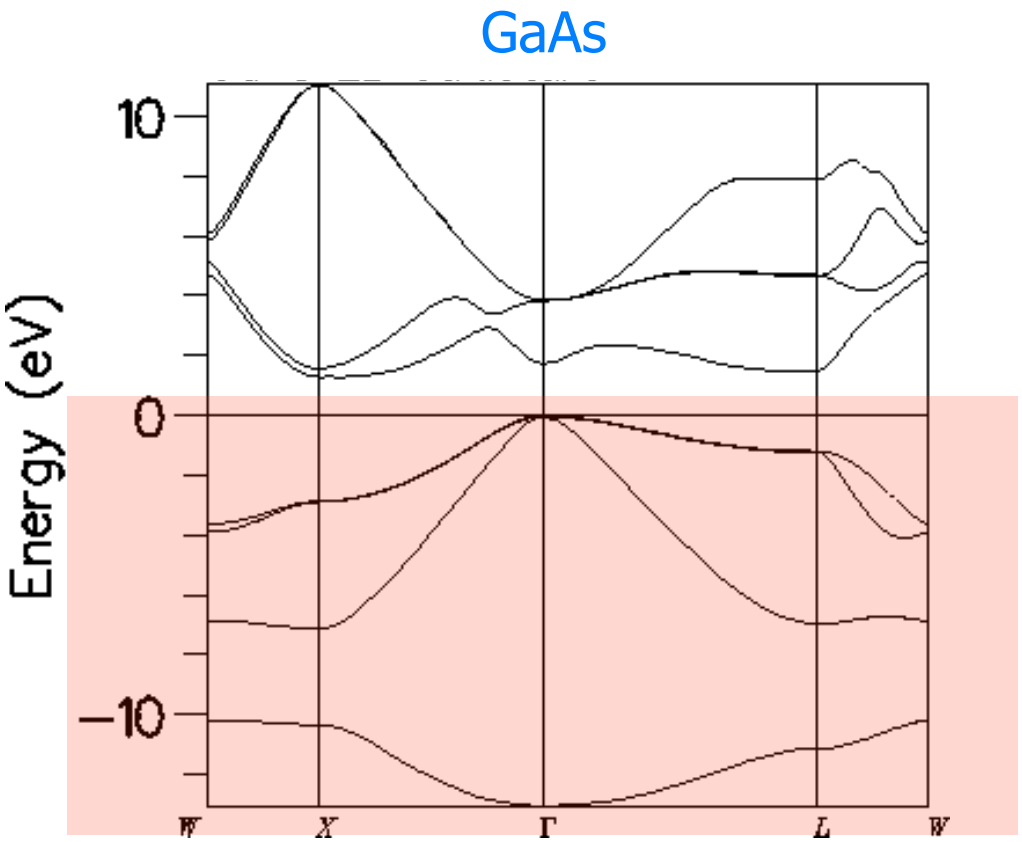
Wannier functions: Si

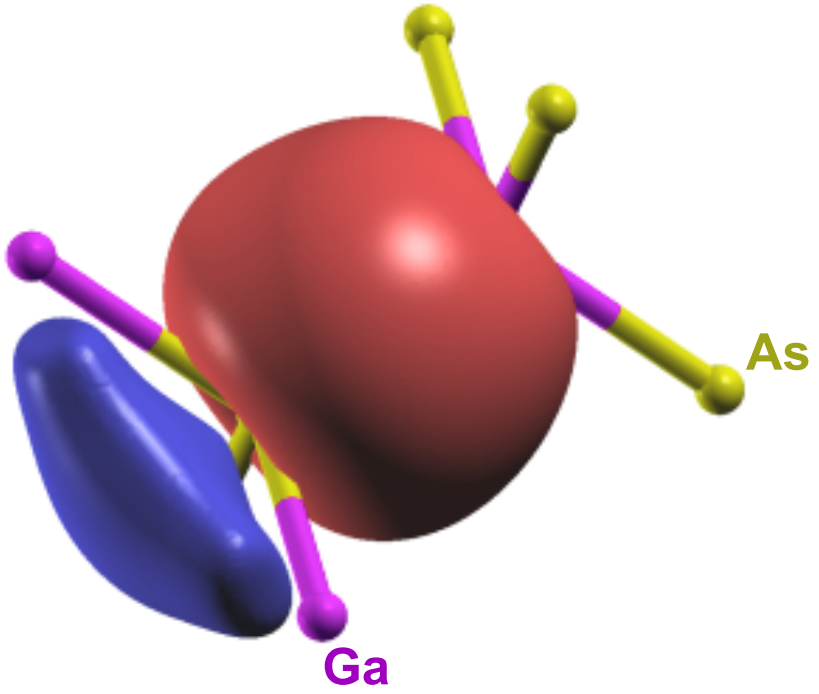
Si



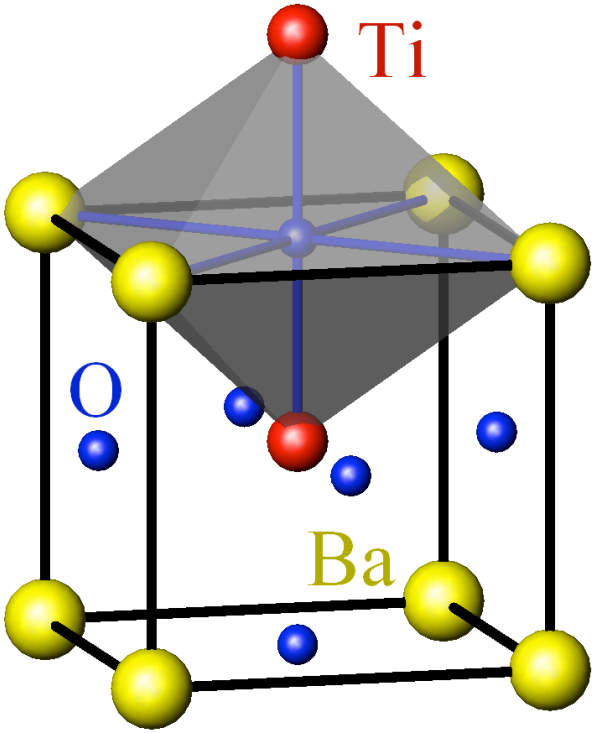


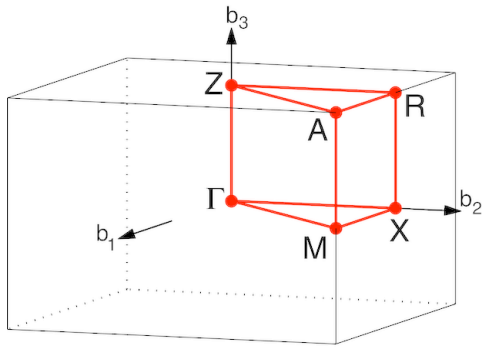
Wannier functions: GaAs

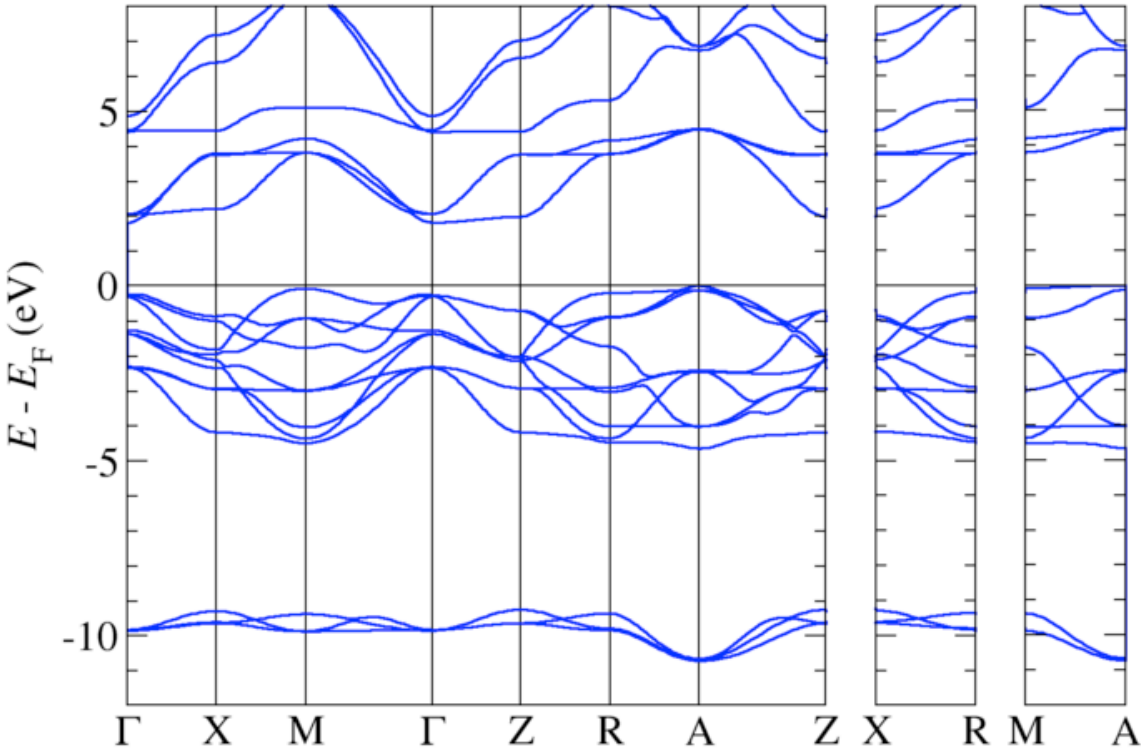




$BaTiO_3$



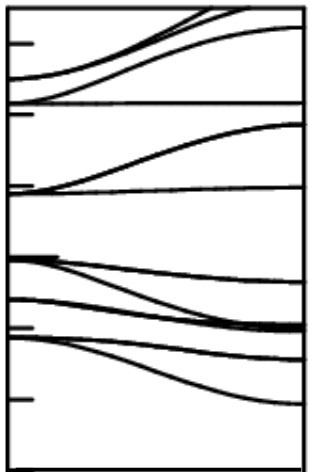




9 bands:
mostly O_{2p}
+ some Ti_{3d}

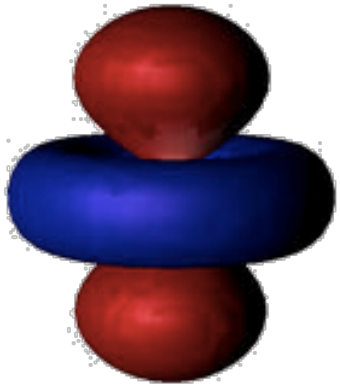
Example: Wannier functions in $BaTiO_3$

$BaTiO_3$

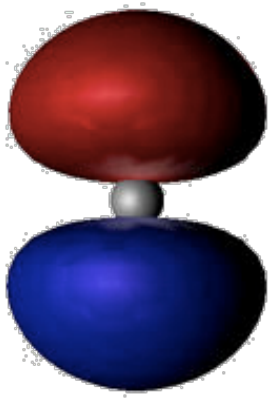


Mainly Ti *3d*
(also some O *2p*)

Mainly O *2p*
(also some Ti *3d*)

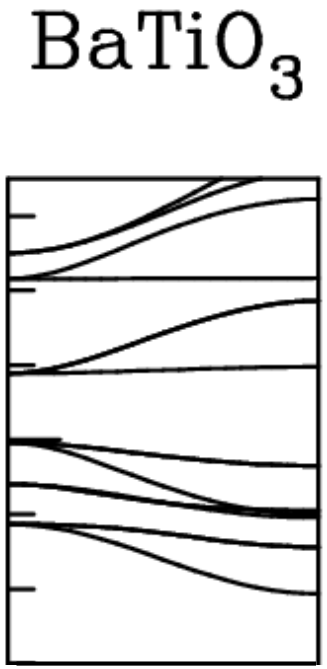


Ti *3d*

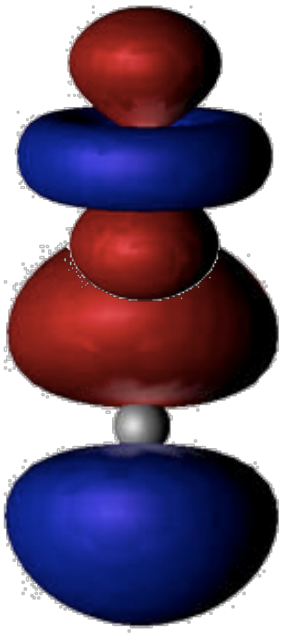


O *2p*

Example: Wannier functions in $BaTiO_3$



Mainly O *2p*
(also some Ti *3d*)



Ti *3d*

O *2p*

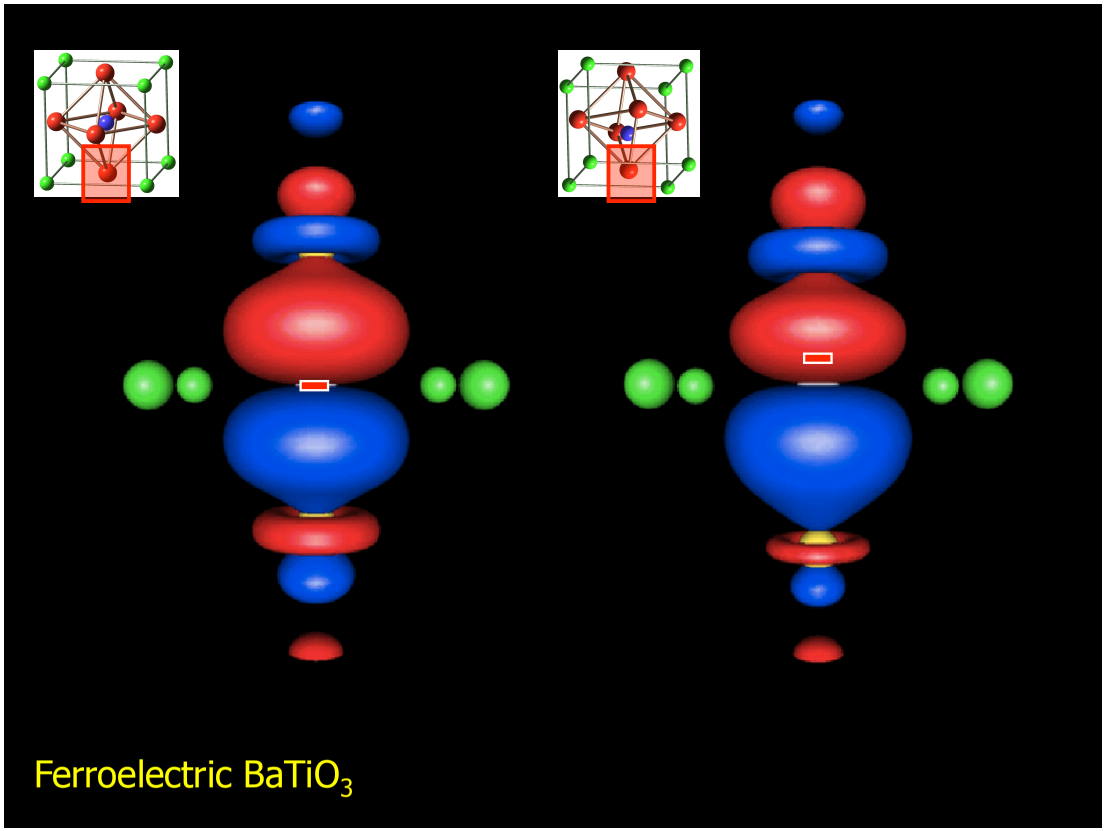


Figure 2: Isosurface contours for a maximally-localized Wannier function in $BaTiO_3$ in the paraelectric (left) and ferroelectric (right) phase. O atoms are in white, Ti yellow, and Ba green. The WF is one of the 9 originating from the composite group of the O $2p$ bands, showing strong and polarizable hybridization between the $2p_z$ orbital of O and the $3d_{z^2}$ orbitals of Ti, usually considered empty in an ionic picture. [From Ref. [19]]