Wannier functions for several classes of materials

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Diamond and zincblende structures

Si (diamond)  GaAs (zincblende)
$sp_3 - sp_3$ bond orbitals

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$sp^3$ methyl radicals

overlap of $sp^3$ orbitals

$C - C$ $\sigma$-bond
Wannier functions in a-Si

Fornari et al.

Fourfold defect in Si

Si atoms are in green, vacancies in black, and the centers of the MLWFs in blue. (Fornari, 2001)
Perovskite crystal structure

Example: Wannier functions in BaTiO$_3$
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BaTiO$_3$

\[
\begin{align*}
\text{Mainly Ti } 3d \\
&\text{(also some O } 2p) \\
\text{Mainly O } 2p \\
&\text{(also some Ti } 3d)
\end{align*}
\]
Paraelectric and ferroelectric state

Paraelectric BaTiO$_3$  Ferroelectric BaTiO$_3$

(Courtesy N. Marzari)
WFs in SrTiO$_3$

Wannier analysis of PVDF polymers and copolymers

Courtesy S. Nakhmanson