Boundary Condition for Electronic Structure of Embedded, Strained Nanostructures
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Question
Which is the efficient boundary condition that eliminates surface states:
(1) periodic, (2) surface-orbital-energy shift,
(3) dangling-bond-energy shift

Main Results
✓ Periodic BC requires a flat boundary and a large supercell.
✓ Surface-orbital-energy shift fails to eliminate some surface states.
✓ Dangling-bond-energy shift eliminates all surface states with a minimal simulation domain.
Boundary Conditions with $sp^3$ tight-binding model

1) Periodic: \[ H \rightarrow H + \sum_{jk} t_{jk} |j \rangle \langle k | \]

2) Surface-Orbital Shift:
\[ H \rightarrow H + \sum_{S} \Delta_S |S \rangle \langle S | \]

\[
\begin{bmatrix}
E_s + \Delta_S & 0 & 0 & 0 \\
0 & E_p + \Delta_S & 0 & 0 \\
0 & 0 & E_p + \Delta_S & 0 \\
0 & 0 & 0 & E_p + \Delta_S \\
\end{bmatrix}
\]

3) Dangling-Bond Shift:
\[ H \rightarrow H + \sum_{D} \Delta_D |D \rangle \langle D | \]

\[
\begin{bmatrix}
E_s + \frac{\Delta_D}{2} & 0 & \frac{\Delta_D}{2} & 0 \\
0 & E_p + \frac{\Delta_D}{2} & 0 & \frac{\Delta_D}{2} \\
\frac{\Delta_D}{2} & 0 & E_p + \frac{\Delta_D}{2} & 0 \\
0 & \frac{\Delta_D}{2} & 0 & E_p + \frac{\Delta_D}{2} \\
\end{bmatrix}
\]
Surface State Elimination

Lanczos Eigenvalue Search

(a) 1.5
(b) 1.5
(c) 1.5

Eigenvalues (eV)

Surface States

Gap

Number of Lanczos Iterations

InAs dot embedded in GaAs

No Boundary Condition

Surface Orbital Shift with $\Delta_S = 5$ eV

Dangling Bond Shift with $\Delta_D = 5$ eV or Periodic Boundary Condition
Buffer Size for Strain Calculation

Strain

Energy Gap

- Small-buffer simulation underestimates the dot strain.
- This leads to a smaller energy gap.
- Large buffer is needed for accurate strain description.
Buffer Truncation for Electronic Structure

- Electron states are localized in the dot.
- Truncating buffer reduces problem size.

- Truncated boundary is bent due to strain.
- Difficult to implement periodic BC.
- Easy to implement non-periodic BC.
Energy Convergence with Truncated Buffer

\[ \Delta E_{\text{electron}} \]

\[ E_{\text{gap}} \]

\[ \Delta E_{\text{hole}} \]

✓ Energies quickly converge as truncated buffer thickness increases.
Energy Sensitivity to Dangling Bond Shift

$E_{e2}$
$E_{e1}$
$E_{h1}$
$E_{h2}$

✓ Eigenvalues are insensitive to the choice of dangling bond shift.