Pseudopotentials: design, testing, typical errors

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Si graphical output – $n(r)$

14_Si.plot Charge Densities

Radius (a_B)

0.836279, 9.86474
Si graphical output – s AE/PS WF

14_Si.plot Wave Functions

S full
S pseudo

$R_C$

2.42929, 1.20330
Si graphical output – excited

14_Si.plot Projector Wave Functions

Radius (a_B)

S1 pseudo
S2 pseudo

2.42929, 1.27051
Si graphical output – logd

Good matching from -2 to +1 Ha important

-1.17234, 9.58359
Si graphical output – convergence error

Decay should be ~linear on this scale

(1 Ha = 2 Ryd = 2*13.6058 eV)
Si test – silicon carbide zinc blende

Calculated Vol = 10.54 \text{ Ang}^3/\text{atom}, B_0=211.1 \text{ GPa}, B’ = 3.90
Reference Vol = 10.50 \text{ Ang}^3/\text{atom}, B_0=212.7 \text{ GPa}, B’ = 3.69

Error (%) 0.36% -0.76% 5.6%
More difficult example – Ti 3d state

22_Ti.plot Ion Pseudopotentials

Radius (a_B)

-0.856718, -12.8548
More difficult example – Ti 3d state

Very localized, poor agreement below $r_c=2.4$ a.u.
More difficult example – Ti 3d state

Error dominated by d state
More difficult example – Ti 3d state

If we decrease $r_c$ to 2.2, we get better agreement...
More difficult example – Ti 3d state

But the convergence is much worse.
We can try to force it lower by adjusting the q target…
More difficult example – Ti 3d state

Warning signs – oscillatory behavior in d-channel
Looks suspicious…
More difficult example – Ti 3d state

We made problem worse!
Cannot solve all problems through optimization

This tradeoff will need to be tested in solid state calcs with application in mind.
Conclusions

- Kohn-Sham equations can be solved
  - All-electron or pseudopotentials

- Pseudopotentials can be made fast and accurate
  - 0.15% lattice constant error, 5% bulk modulus, only slightly worse than all-electron

- Careful testing is required
  - Different structures, oxidation states
  - Tradeoffs between accuracy and speed – depends on application

- GBRV library provides good speed/accuracy combination

- In rest of lab, you will design/test pseudopotentials…
Lab

- INSTRUCTIONS.txt in nanohub
  - Or www.physics.rutgers.edu/~kgarrity/INSTRUCTIONS.txt

1. Aluminum – Run psp generator, test in 2 structures
2. Boron – Adjust $r_c$ to be more accurate/harder, re-test
3. Indium – Compare without/with semicore d state to potential, test

5. Phosphorous – optional. Create input file from Al.