Constructing Pseudopotentials with the Program

fhi98PP

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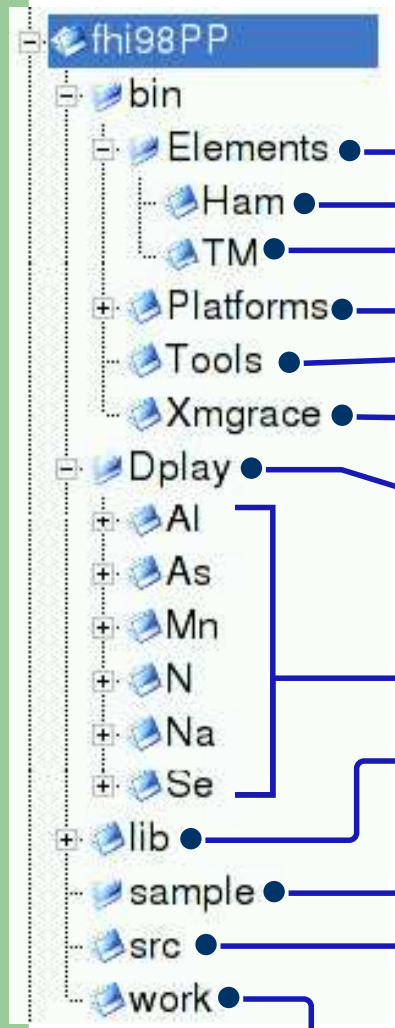
Demonstration Session D1

Intro to fhi98PP

Guide to the directories: fhi98PP/*



Database of input files (do not use uncritically!)

for Hamann type pseudopotentials

for Troullier-Martins type pseudopotentials

Platform-specific resources

Backup for shell scripts [. . . psgen, pswatch]

Header files for Xmgrace-compatible graphics output

Hands-on tour's prepared playground with examples

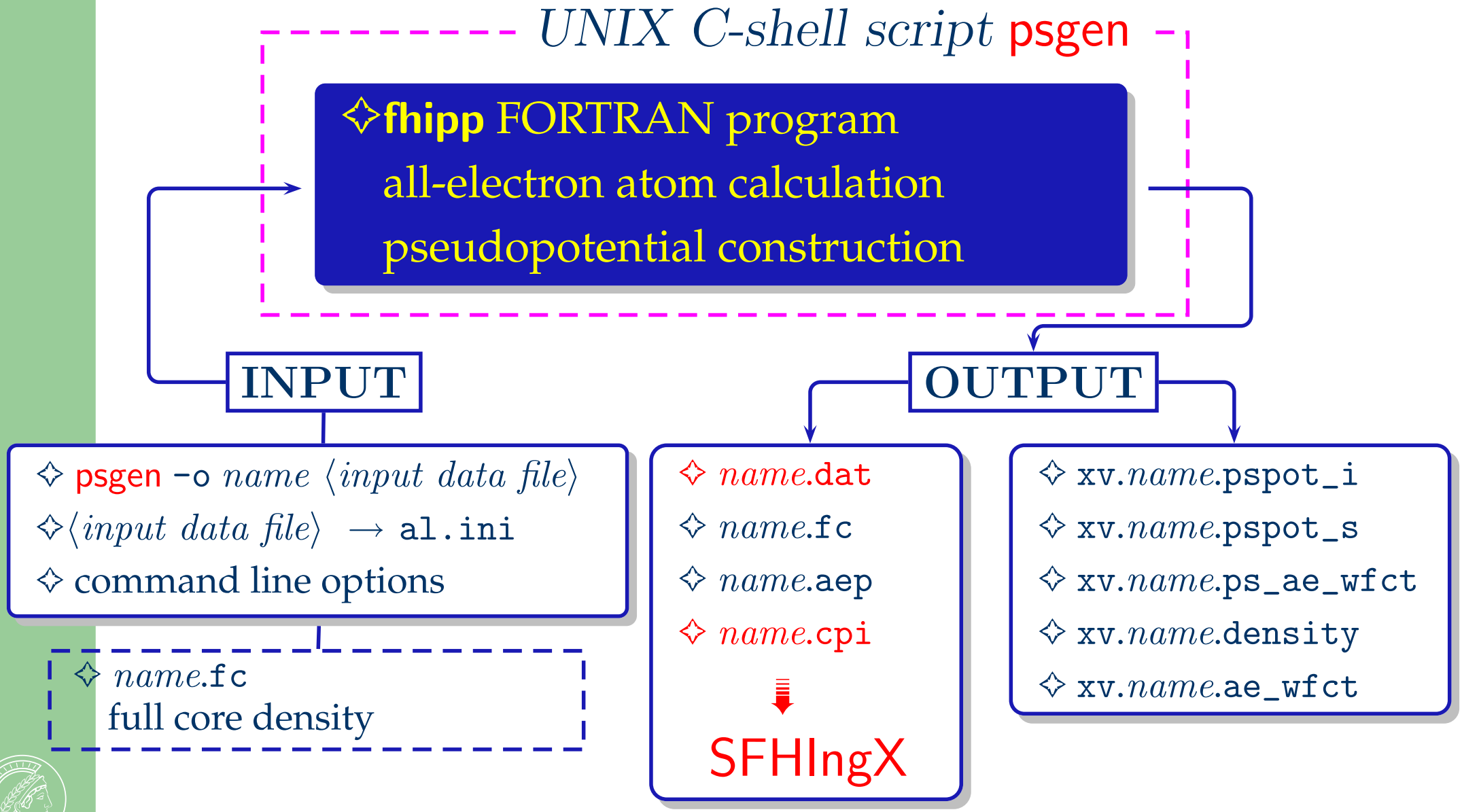
Archive of selected LAPACK routines (used as "*libFree.a*")

Sample run

Makefile and FORTRAN source files

Testing ground

The psgen tool



The pswatch tool

UNIX C-shell script pswatch

plsp FORTRAN program

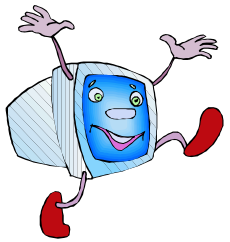
pseudo atom calculation
ghost state analysis
logarithmic derivatives
plane-wave convergence test

INPUT

- pswatch -i *name* ⟨*input data file*⟩
- ⟨*input data file*⟩ → `al.ini`
- command line options
- *name*`.cpi`
  ionic pseudopotentials
- *name*`.aep`
  all-electron potential

OUTPUT

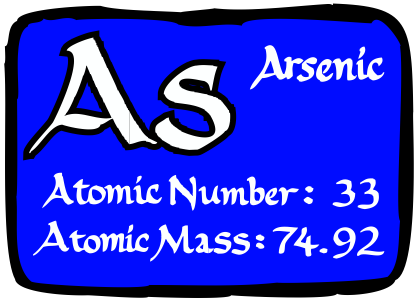
- Terminal



- *name*`.test`

- `xv.`*name*`.lder`
- `xv.`*name*`.pspot_i`
- `xv.`*name*`.pspot_s`

Xmgrace



Transferability of fully separable potentials

.../fhi98PP/Dplay/As

.../E1/As

Steps

1. Generate a Hamann type pseudopotential for As

   `psgen -xv -o as as.ini`

   - -xv : skip graphics output
   - -o as : identifying prefix for output files
   - as.ini : input data file

2. Identifying a ghost state for the fully separable form of the pseudopotential

   `pswatch -i as as.ini -l 2`

   - -i as : identifying prefix for input/output files
   - -l 2 : angular momentum for local pseudopotential, $l_{\mathrm{loc}} = 2$

3. More options : `-h, -v, -rs, -rd ...`

Input file format (*.ini)

```
33.00   6  2   8   0.00   : z nc nv iexc rnlc
        1  0     2.00     : n(i) l(i) f(i)
        2  0     2.00     :
        2  1     6.00     :
        3  0     2.00     :
        3  1     6.00     :
        3  2    10.00     :
        4  0     2.00     :
        4  1     3.00     :
  2  h                    : lmax s_pp_def
  0  1.25  0.00 h         : lt  rct  et  s_pp_type
  2  2.05  0.00 h         :
```

optional input, psgen only

$_{33}$As

$1s^2$
$2s^2$
$2p^6$
$3s^2$
$3p^6$
$3d^{10}$
$4s^2$
$4p^3$

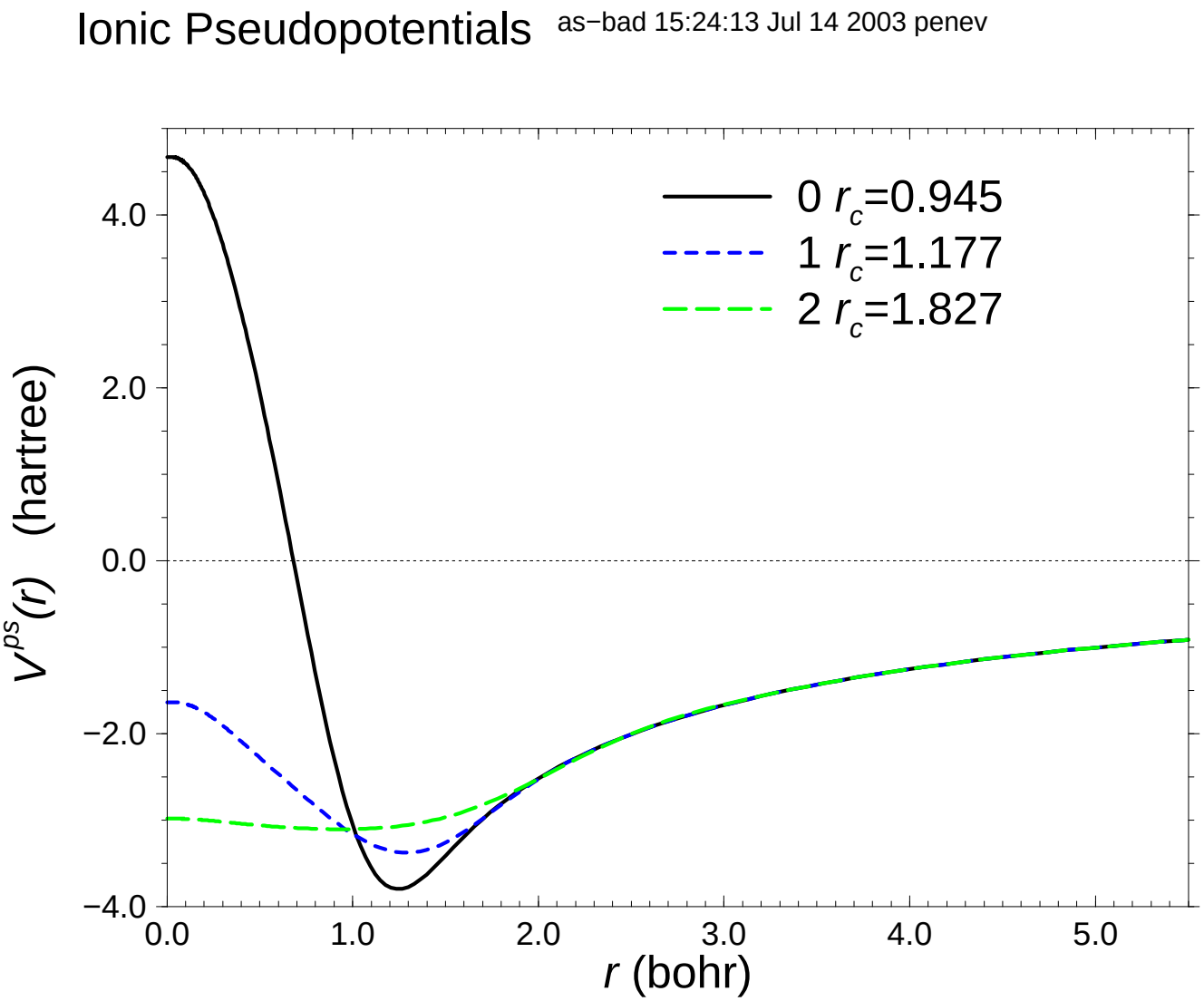
❶ psgen -o as-bad as.ini

as-bad.dat

```
 .....
    === HAMANN mode ===   h

  l  n     radius:     node      peak      default core
x 0  4                 0.723     1.578     0.947
x 1  4                 0.778     1.966     1.179
x 2  4                 0.000     0.000     1.864

        === pseudo atom ===

l  type  rcore       rmatch          eigenvalue(eV)      norm test   slope test
                                 all-electron     pseudo
0  h     0.9454249   2.3894777 -14.6997676 -14.6997681   1.0000000   1.0000064
1  h     1.1775996   3.1251228  -5.3417404  -5.3417406   1.0000000   1.0000050
2  h     1.8270014   4.5062796  -5.3417404  -5.3417405   1.0000000   1.0000000
.....
```

❶ psgen -o as-bad as.ini

xv.as-bad.pspot_i



❷ pswatch -i as-bad as.ini -l 2

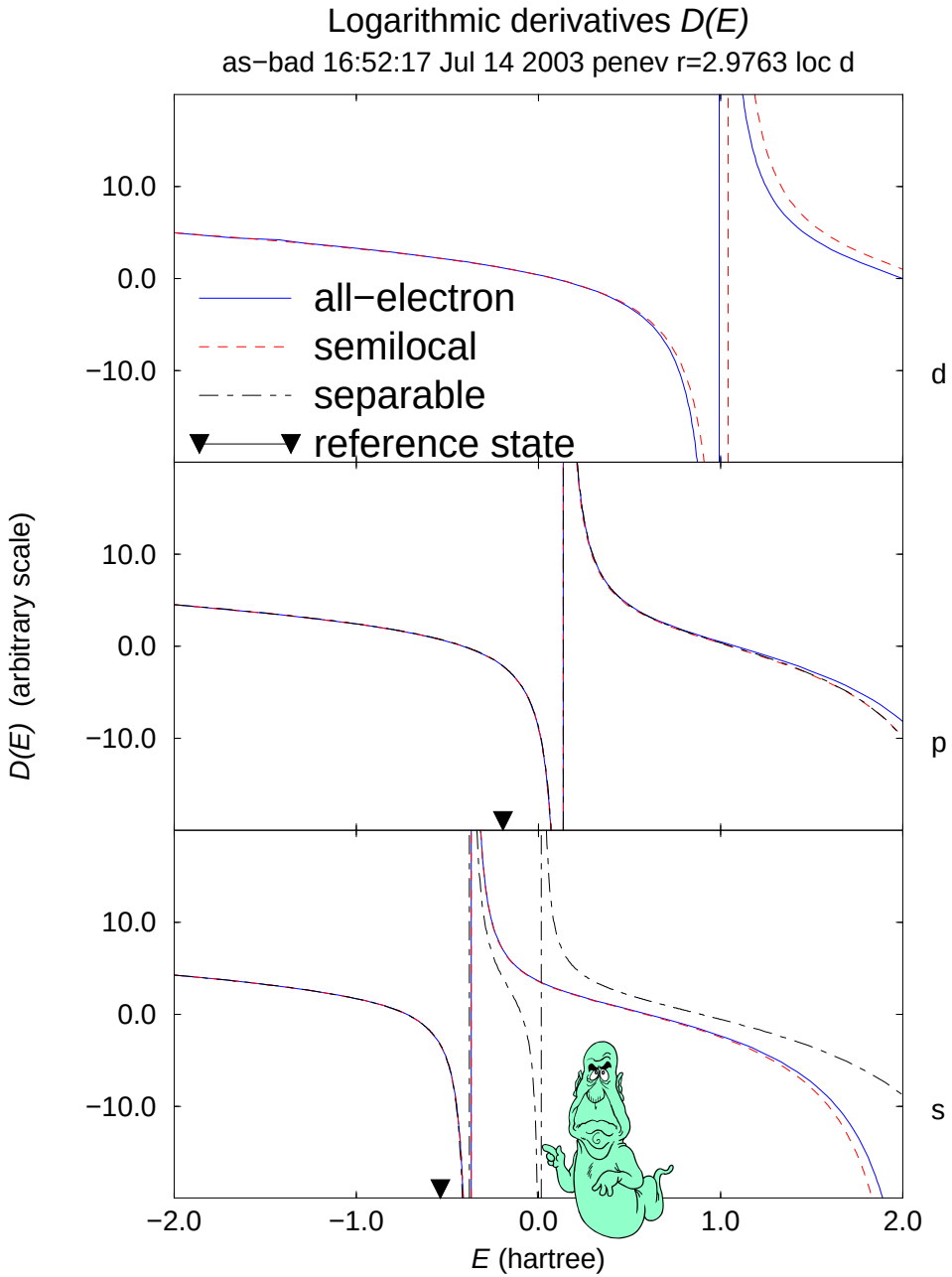
as-bad.test

```
.....
 --- kb potentials: spectrum of bound states (eV) ---

             l          e0          e1          e2
semilocal    0     -14.6998     -0.4194      0.0000
nonlocal     0     -14.6998     -2.3989      0.0000
.....
 --- analysis of kb potentials: s waves  ---

 * no ghost (ekb < 0, eref < eloc0)

                      kb cosine      -0.1710
                      kb energy     -93.3053 eV      ekb
   local potential groundstate     -14.1903 eV    eloc0
        dto. 1st excited state      -0.5969 eV    eloc1
              reference energy     -14.6998 eV     eref

.....
```

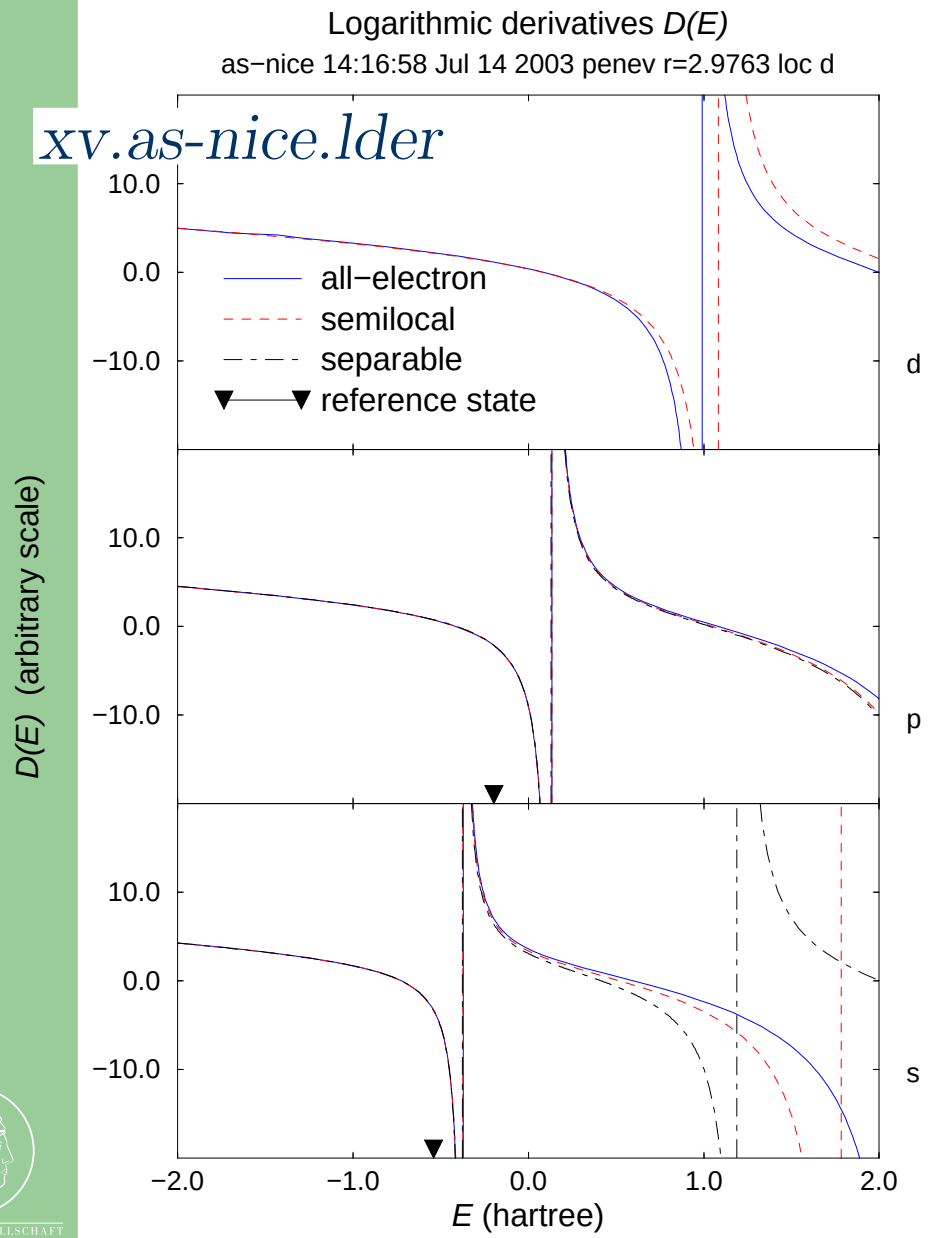
❷ pswatch -i as-bad as.ini -l 2

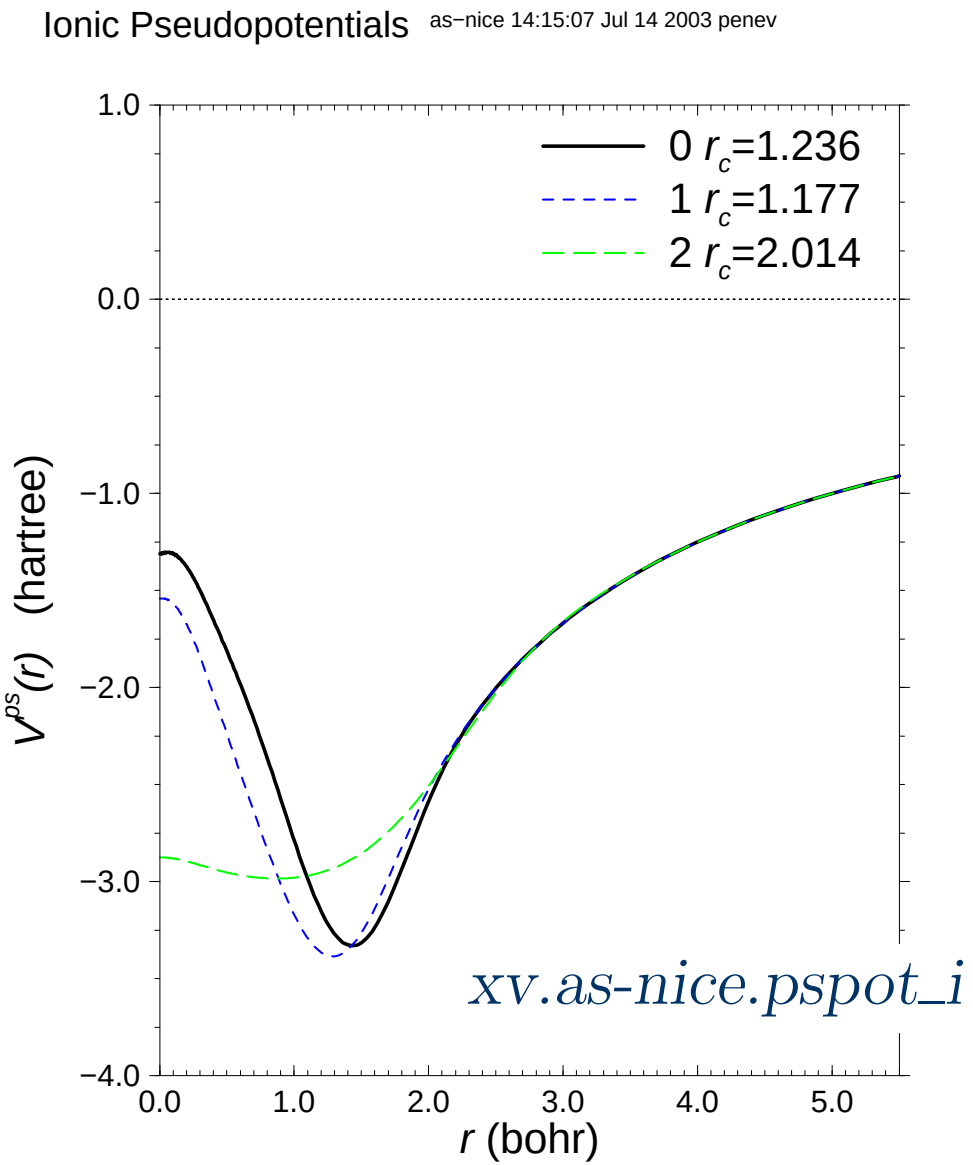
xv.as-bad.lder

$$D_l(E, r^{\mathrm{diag}}) = \left.\frac{d}{dr} \ln u_l(E;r)\right|_{r^{\mathrm{diag}}}$$



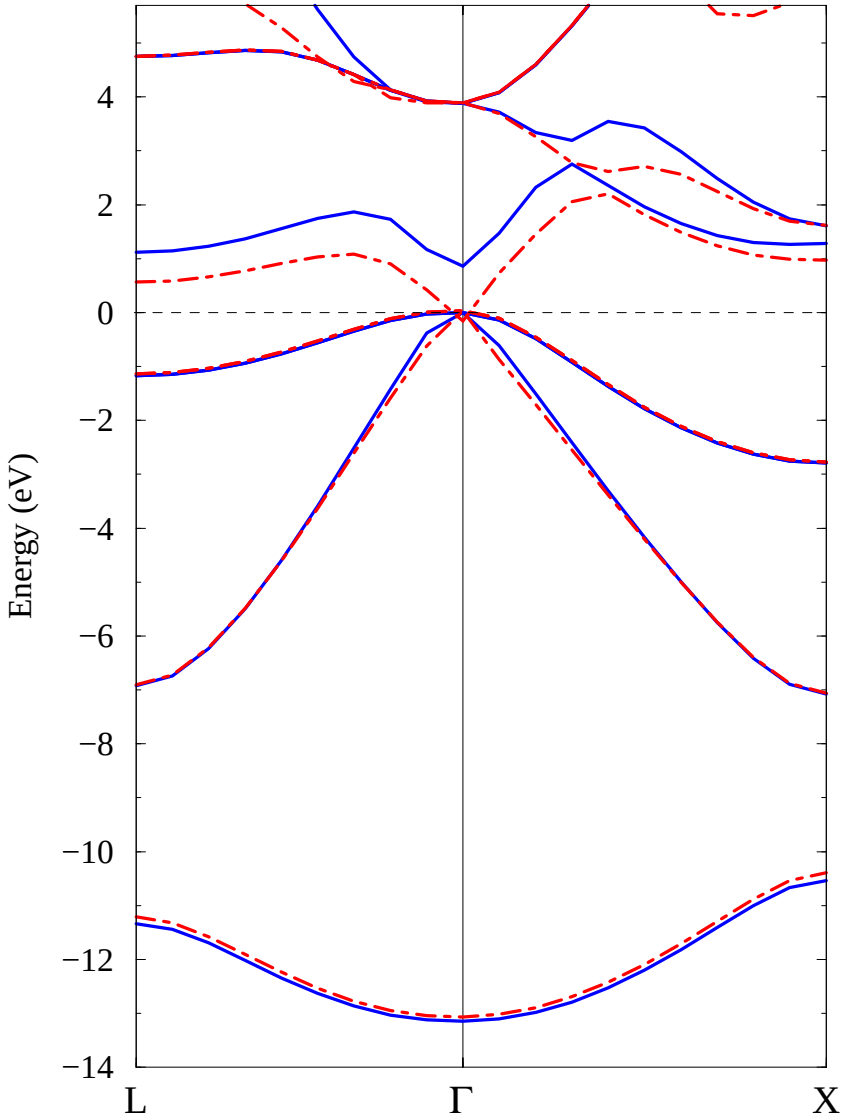
❶ psgen -v -o as-nice as.ini -rs 1.25 -rd 2.05





The evil a ghost state can do...

- GaAs bulk band structure



as-nice.cpi (no ghost)

LDA	no ghost	with ghost
a_0	5.54 Å	5.54 Å
E_{gap}	0.9 eV	∅

Tasks to do:

☞ Generate and assess pseudopotentials for

❶ Al ..... Getting familiar with fhi98PP

❷ Na ..... Nonlinear core-valence exchange-correlation

❸ As ..... Transferability of fully separable potentials

❹ Se ..... Analysis and removal of ghost states

❺ Mn ..... Local potential for *d* elements – Spin polarization

❻ N ..... Plane-wave convergence

3 points to note. . .

- Lectures L4 & L8 by Martin Fuchs
- M. Fuchs and M. Scheffler, *Comput. Phys. Commun.* 119, 67–98 (1999)
- www.fhi-berlin.mpg.de/th/fhi98md/fhi98PP/