

All electron calculations, comparing to the ld1.x code of Quantum Espresso

```
[1] import numpy as np
import matplotlib.pyplot as plt
import subprocess

# add pstudio to the search path
import sys
sys.path.append('..')
```



```
[2] from pstudio import AE, set_output
from pstudio.configuration import *
```

```
[3] def ld1_create_input(atom, xcname='pz'):
    el = Element(atom)
    z = el.get_atomic_number()
    conf = el.get_configuration()

    ld1_in = """&input
    title = '{0}'
    prefix = '{0}'
    zed = {1}
    dft = '{2}'
    config = '{3}'
    rel = 1
    iswitch = 1
    beta = 0.2
    xmin = -8.0, dx = 0.005
    /""".format(atom, z, xcname, conf)
    return ld1_in

def ld1_run(inp, ld1='/home/ceresoli/Codes/q-e/bin/ld1.x'):
    p = subprocess.Popen(ld1, stdin=subprocess.PIPE,
    stdout=subprocess.PIPE)
    p.stdin.write(bytes(inp, encoding='ascii'))
    out = p.communicate()[0]
    p.stdin.close()
    return str(out, encoding='ascii')

def ld1_get_etot(out):
    pos1 = out.find('Etot') + 6
```

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pos2 = out.find(',', pos1) - 3
etot = float(out[pos1:pos2])
return etot/2.0 # rydberg to hartree

```

```

[4] def pstudio_etot(atom, xcname='lda'):
    set_output(None)
    ae = AE(atom, xcname)
    ae.run()
    return ae.Etot

def ld1_etot(atom, xcname='pz'):
    inp = ld1_create_input(atom, xcname)
    out = ld1_run(inp)
    return ld1_get_etot(out)

```

```

[8] print('=====')
    print('Atom          PStudio          LD1')
    print('Abs.err.  Rel.err.')
    print('=====')
    for atom in atom_table:
        pst = pstudio_etot(atom)
        ld1 = ld1_etot(atom)
        aerr = abs(pst-ld1)
        rerr = abs(pst-ld1)/abs(ld1) * 100
        print('{0:2s} {1:18.6f} {2:18.6f} {3:18.6f} {4:8.4f}%'.format(atom, pst, ld1, aerr, rerr))

```

```

=====
Atom          PStudio          LD1          Abs.err.  Rel.err.
=====
H             -0.445896         -0.445899         0.000003   0.0006%
He            -2.834423         -2.834419         0.000004   0.0001%
Li            -7.334881         -7.334878         0.000003   0.0000%
Be           -14.449031        -14.449025         0.000006   0.0000%
B            -24.350610        -24.350603         0.000007   0.0000%
C            -37.440489        -37.440480         0.000009   0.0000%
N            -54.053911        -54.053902         0.000009   0.0000%
O            -74.524978        -74.524969         0.000009   0.0000%
F           -99.186849        -99.186840         0.000009   0.0000%
Ne          -128.372234        -128.372226         0.000008   0.0000%
Na          -161.652814        -161.652805         0.000009   0.0000%
Mg          -199.453675        -199.453666         0.000009   0.0000%
Al          -241.763848        -241.763838         0.000010   0.0000%
Si          -288.819834        -288.819825         0.000008   0.0000%
P           -340.787121        -340.787112         0.000008   0.0000%
S           -397.830714        -397.830704         0.000010   0.0000%
Cl          -460.115597        -460.115587         0.000010   0.0000%

```

Ar	-527.807210	-527.807200	0.000010	0.00000%
K	-600.556323	-600.556320	0.000003	0.00000%
Ca	-678.689044	-678.689052	0.000008	0.00000%
Sc	-762.317250	-762.317240	0.000010	0.00000%
Ti	-851.721779	-851.721771	0.000008	0.00000%
V	-947.058353	-947.058344	0.000008	0.00000%
Cr	-1048.477666	-1048.477657	0.000009	0.00000%
Mn	-1156.138132	-1156.138123	0.000008	0.00000%
Fe	-1270.185387	-1270.185380	0.000007	0.00000%
Co	-1390.773818	-1390.773812	0.000006	0.00000%
Ni	-1518.056143	-1518.056135	0.000008	0.00000%
Cu	-1652.259260	-1652.259251	0.000009	0.00000%
Zn	-1793.316255	-1793.316249	0.000006	0.00000%
Ga	-1941.118397	-1941.118391	0.000006	0.00000%
Ge	-2095.896421	-2095.896415	0.000006	0.00000%
As	-2257.750916	-2257.750910	0.000005	0.00000%
Se	-2426.787202	-2426.787199	0.000003	0.00000%
Br	-2603.113693	-2603.113690	0.000003	0.00000%
Kr	-2786.841182	-2786.841181	0.000001	0.00000%
Rb	-2977.644308	-2977.644306	0.000001	0.00000%
Sr	-3175.814495	-3175.814498	0.000002	0.00000%
Y	-3381.387196	-3381.387200	0.000004	0.00000%
Zr	-3594.596566	-3594.596569	0.000003	0.00000%
Nb	-3815.544823	-3815.544829	0.000006	0.00000%
Mo	-4044.418082	-4044.418092	0.000009	0.00000%
Tc	-4281.257579	-4281.257589	0.000011	0.00000%
Ru	-4526.277052	-4526.277065	0.000013	0.00000%
Rh	-4779.500070	-4779.500088	0.000018	0.00000%
Pd	-5041.131076	-5041.131099	0.000022	0.00000%
Ag	-5311.132659	-5311.132685	0.000025	0.00000%
Cd	-5589.609856	-5589.609881	0.000026	0.00000%
In	-5876.445886	-5876.445918	0.000032	0.00000%
Sn	-6171.866193	-6171.866235	0.000042	0.00000%
Sb	-6475.967318	-6475.967361	0.000043	0.00000%
Te	-6788.848779	-6788.848829	0.000050	0.00000%
I	-7110.612540	-7110.612598	0.000058	0.00000%
Xe	-7441.362823	-7441.362887	0.000064	0.00000%
Cs	-7780.834486	-7780.834568	0.000081	0.00000%
Ba	-8129.312306	-8129.312394	0.000088	0.00000%
La	-8486.873997	-8486.874090	0.000094	0.00000%
Ce	-8853.888352	-8853.888458	0.000107	0.00000%
Pr	-9230.606283	-9230.606406	0.000122	0.00000%
Nd	-9617.099256	-9617.099394	0.000138	0.00000%
Pm	-10013.517934	-10013.518092	0.000158	0.00000%
Sm	-10419.999611	-10419.999788	0.000176	0.00000%
Eu	-10836.682999	-10836.683199	0.000201	0.00000%
Gd	-11263.568390	-11263.568600	0.000210	0.00000%
Tb	-11701.218619	-11701.218858	0.000239	0.00000%
Dy	-12149.357756	-12149.358024	0.000268	0.00000%
Ho	-12608.272767	-12608.273061	0.000294	0.00000%
Er	-13078.112875	-13078.113195	0.000320	0.00000%
Tm	-13559.029898	-13559.030263	0.000365	0.00000%

Yb	-14051.178370	-14051.178775	0.000405	0.00000%
Lu	-14554.526672	-14554.527134	0.000462	0.00000%
Hf	-15069.205193	-15069.205705	0.000512	0.00000%
Ta	-15595.349551	-15595.350125	0.000573	0.00000%
W	-16133.101534	-16133.102171	0.000637	0.00000%
Re	-16682.608474	-16682.609182	0.000708	0.00000%
Os	-17244.022902	-17244.023697	0.000795	0.00000%
Ir	-17817.502406	-17817.503290	0.000884	0.00000%
Pt	-18403.243742	-18403.244733	0.000991	0.00000%
Au	-19001.370831	-19001.371935	0.001105	0.00000%
Hg	-19611.982401	-19611.983633	0.001233	0.00000%
Tl	-20234.978755	-20234.980143	0.001387	0.00000%
Pb	-20870.700602	-20870.702153	0.001551	0.00000%
Bi	-21519.318707	-21519.320439	0.001732	0.00000%
Po	-22181.011640	-22181.013584	0.001943	0.00000%
At	-22855.965229	-22855.967400	0.002171	0.00000%
Rn	-23544.372644	-23544.375084	0.002440	0.00000%
Fr	-24246.103662	-24246.106404	0.002742	0.00000%
Ra	-24961.538407	-24961.541479	0.003072	0.00000%
Ac	-25690.821194	-25690.824646	0.003452	0.00000%
Th	-26434.265417	-26434.269302	0.003884	0.00000%
Pa	-27192.268224	-27192.272601	0.004377	0.00000%
U	-27965.110717	-27965.115655	0.004937	0.00000%
Np	-28753.058224	-28753.063801	0.005577	0.00000%
Pu	-29556.456485	-29556.462788	0.006303	0.00000%
Am	-30375.493708	-30375.500844	0.007135	0.00000%