A cubic spline solver for generalized density functional treatments of atoms and the generation of atomic datasets for use with exchange-correlation functionals including the meta generalized gradient approximation

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I. SAMPLE INPUT FILES USED IN THIS PAPER

A. Inputs for atompaw version 4.2.0.0

Note that these inputs produce atomic data sets in XML format used in ABINIT. Atomic data sets in UPF format used in QUANTUM ESPRESSO are not quite yet compatible for meta-GGA functionals.

```
-----------------------Si PBE  (libxc)-----------------------------
Si 14
GGA_X_PBE+GGA_C_PBE splineinterp loggrid    2001
3 3 0 0 0 0
3 1 2
0 0 0
c
c
v
c
v
2
1.7   1.5   1.7    1.7
y
14
n
y
14
n
y
2
y
12
n
MODRRKJ VANDERBILTORTHO  Besselshape
3 0   VPSMATCHNC
1.7
1.7
1.7
1.7
1.7
1.7
ABINITOUT
default
XMLOUT
default
PWSCFOUT
UPFDX  0.0125d0   UPFXMIN   -7.d0     UPFZMESH 14.d0
PWPAWOUT
END
------------------------------------------------------------


----------------Si r2SCAN01-----------------------------------
Si 14
MGGA-R2SCAN-01  splineinterp   loggrid    2001
3 3 0 0 0 0
3 1 2
0 0 0
c
```

```
c
v
c
v
2
1.7   1.5   1.7    1.7
y
14
n
y
14
n
y
2
y
12
n
MODRRKJ VANDERBILTORTHO  Besselshape
3 0   VPSMATCHNC
1.7
1.7
1.7
1.7
1.7
1.7
ABINITOUT
default
XMLOUT
default
PWSCFOUT
UPFDX  0.0125d0   UPFXMIN   -7.d0     UPFZMESH 14.d0
PWPAWOUT
END
------------------------------------------------------------

----------------------Si r2SCAN01 (libxc)------------------
Si 14
WTAU  XC_MGGA_X_R2SCAN01+XC_MGGA_C_R2SCAN01   loggrid    2001
3 3 0 0 0 0
3 1 2
0 0 0
c
c
v
c
v
2
1.7   1.5   1.7    1.7
y
14
n
y
14
n
y
2
y
12
n
MODRRKJ VANDERBILTORTHO  Besselshape
3 0   VPSMATCHNC
1.7
1.7
```

```
1.7
1.7
1.7
1.7
ABINITOUT
default
XMLOUT
default
PWSCFOUT
UPFDX  0.0125d0   UPFXMIN   -7.d0     UPFZMESH 14.d0
PWPAWOUT
END
------------------------------------------------------------

-------------Na  r2SCAN  (libxc) --------------------------
Na 11
WTAU  XC_MGGA_X_R2SCAN+XC_MGGA_C_R2SCAN   loggrid    2001
3 2 0 0 0 0
3 0 1
0 0 0
c
v
v
v
1
1.7   1.5   1.7    1.7
n
y
4.6
n
MODRRKJ VANDERBILTORTHO  Besselshape
2 0   VPSMATCHNC
1.5
1.7
1.5
1.7
ABINITOUT
default
XMLOUT
default
PWSCFOUT
UPFDX  0.0125d0   UPFXMIN   -7.d0     UPFZMESH 11.d0
PWPAWOUT
END
------------------------------------------------------------------
```

B. Inputs for abinit version 9.6.2

```
---------------NaCl  r2SCAN   from r2SCAN datasets -- abi format ------
#  NaCl
#
#Convergence parameters
ecut 40.00
pawecutdg 40.
chkprim 0
ndtset 13
acell1 3*10.2
acell2 3*10.3
acell3 3*10.4
acell4 3*10.5
```

```
acell5 3*10.6
acell6 3*10.7
acell7 3*10.8
acell8 3*10.9
acell9 3*11.0
acell10 3*11.1
acell11 3*11.2
acell12 3*11.3
acell13 3*11.4
rprim  0.0  0.5  0.5
       0.5  0.0  0.5
       0.5  0.5  0.0
nstep 60
toldfe 1.0d-8
occopt 7 tsmear 5.0d-4
#Definition of the atom types
ntypat 2
znucl 11 17
#Definition of the atoms
natom 2
typat 1  2
xred
     0.0000000000000000 0.0000000000000000  0.000000000000000
     0.5000000000000000 0.5000000000000000  0.500000000000000
#Definition of the k-point grid
kptopt 1
ngkpt 16 16 16
nshiftk 4
shiftk 0.5 0.5 0.5
  0.5 0.0 0.0
  0.0 0.5 0.0
  0.0 0.0 0.5
prtden 0
### special for mgga
usekden 1
optforces 0
prtwf 1
getwfk -1

pp_dirpath "/Specify/your/data_set_directory/path/here/"
pseudos "Na/r2scan-libxc/Na.MGGA_X_R2SCAN+MGGA_C_R2SCAN-paw.xml,
   Cl/r2scan-libxc/Cl.MGGA_X_R2SCAN+MGGA_C_R2SCAN-paw.xml"
------------------------------------------------------------------------

---------------NaCl  r2SCAN   from PBE datasets -- abi format ------
#  NaCl
#
#Convergence parameters
ecut 40.00
pawecutdg 40.
chkprim 0
ndtset 13
acell1 3*10.2
acell2 3*10.3
acell3 3*10.4
acell4 3*10.5
acell5 3*10.6
acell6 3*10.7
acell7 3*10.8
acell8 3*10.9
acell9 3*11.0
acell10 3*11.1
acell11 3*11.2
```

```
acell12 3*11.3
acell13 3*11.4
rprim  0.0  0.5  0.5
       0.5  0.0  0.5
       0.5  0.5  0.0
nstep 60
toldfe 1.0d-8
occopt 7 tsmear 5.0d-4
#Definition of the atom types
ntypat 2
znucl 11 17
#Definition of the atoms
natom 2
typat 1  2
xred
     0.0000000000000000 0.0000000000000000  0.000000000000000
     0.5000000000000000 0.5000000000000000  0.500000000000000
#Definition of the k-point grid
kptopt 1
ngkpt 16 16 16
nshiftk 4
shiftk 0.5 0.5 0.5
  0.5 0.0 0.0
  0.0 0.5 0.0
  0.0 0.0 0.5
prtden 0
### special for mgga
usekden 1
optforces 0
prtwf 1
getwfk -1
### specify exchange-correlation functional from libxc ID's
ixc=-497498

pp_dirpath "/Specify/your/data_set_directory/path/here/"
pseudos "Na/pbe/Na.GGA_X_PBE+GGA_C_PBE-paw.xml,
    Cl/pbe/Cl.GGA_X_PBE+GGA_C_PBE-paw.xml"
-------------------------------------------------------------------------
```