

Supplementary Information
Corvus: A framework for interfacing scientific software
for spectroscopic and materials science applications

S. M. STORY,^a F. D. VILA,^{a,b*} J. J. KAS,^{a,b} K. B. RANIGA,^c

C. D. PEMMARAJU^b AND J. J. REHR^{a,b}

^a*Department of Physics, University of Washington, Seattle, WA 98195, USA,*

^b*Theory Institute for Materials and Energy Spectroscopies, SLAC National
Accelerator Laboratory, Menlo Park, CA 94025, USA, and* ^c*School of Humanities &
Sciences, Stanford University, Stanford, CA 94305, USA. E-mail: fdv@uw.edu*

```
target_list {
s2
}

usehandlers { Abinit Dmdw }

cell_scaling_abc {
10.68394459291 10.68394459291 10.68394459291
}

cell_vectors {
0.0 0.5 0.5
0.5 0.0 0.5
0.5 0.5 0.0
}

cell_struct_xyz_red {
Ga -0.125 -0.125 -0.125
As 0.125 0.125 0.125
}

mac_diel_const 1.0E+06
pw_encut 30.0
pspfiles {
Ga 31-Ga.LDA.fhi
As 33-As.LDA.fhi
}
nkpoints {
8 8 8
}
nqpoints {
4 4 4
}

dmdw.paths {
1
2 1 0 3.0
2 2 0 3.0
}

dmdw.tempgrid {
300 1.0 300.0
}

dmdw.nlanc 8
```

Supplementary Fig. 1. Example input file for the calculation of the EXAFS Debye-Waller (DW) factors of GaAs, using ABINIT to generate the dynamical matrix, and DMDW to compute the DW factors.

```
acell 10.6839445929 10.6839445929 10.6839445929
ecut 10.0
kptopt 1
natom 2
ngkpt 4 4 4
nshiftk 1
ntypat 2
prtvol -1
rprim 0.0 0.5 0.5
      0.5 0.0 0.5
      0.5 0.5 0.0
shiftk 0
       0
       0
toldfe 0.1
typat 1
      2
xred -0.125 -0.125 -0.125
      0.125 0.125 0.125
znucl 31
      33
```

Supplementary Fig. 2. ABINIT input automatically generated by Corvus from the Corvus input shown in Supp. Fig. 1. This information is used to automatically create a symmetry-adapted q-point grid for the calculation of the dynamical matrix. Other input files, such as the ABINIT “files” definition file are not shown.

```

acell 10.6839445929 10.6839445929 10.6839445929
diemac 12.0E+00
ecut 60.0
getden2 1
getwfk 2
getwfk1 0
getwfk2 0
iscf2 -3
istwfk *1
ixc 7
kptopt 3
kptopt1 1
natom 2
ndtset 10
ngkpt 4 4 4
nline1 8
nqpt 1
nqpt1 0
nqpt2 0
nshiftk 4
nstep 800
ntypat 2
prepgkk 1
prtden1 1
prtgkk 1
prtwf 0
prtwf2 1
qpt10 -2.50000000E-01 5.00000000E-01 2.50000000E-01
qpt3 0.00000000E+00 0.00000000E+00 0.00000000E+00
qpt4 2.50000000E-01 0.00000000E+00 0.00000000E+00
qpt5 5.00000000E-01 0.00000000E+00 0.00000000E+00
qpt6 2.50000000E-01 2.50000000E-01 0.00000000E+00
qpt7 5.00000000E-01 2.50000000E-01 0.00000000E+00
qpt8 -2.50000000E-01 2.50000000E-01 0.00000000E+00
qpt9 5.00000000E-01 5.00000000E-01 0.00000000E+00
rfatpol 1 2
rfdir 1 1 1
rfphon 1
rfphon1 0
rfphon2 0
rprim 0.0 0.5 0.5
      0.5 0.0 0.5
      0.5 0.5 0.0
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
tolvrs 1.0e-10
tolvrs1 1.0d-18
tolwfr2 1.0d-22
typat 1
      2
xred -0.125 -0.125 -0.125
      0.125 0.125 0.125
znucl 31
      33

```

Supplementary Fig. 3. ABINIT input automatically generated by Corvus from the Corvus input shown in Supp. Fig. 1, and from the output of the calculation shown in Supp. Fig 2 (“qpt” entries in the input file). This information is used to automatically create the ABINIT second derivative database files for the calculation of the dynamical matrix. Other input files, such as the ABINIT “files” definition file, and the input file for the merging of the databases are not shown.

```
asr 2
atifc 1 2
elphflag 1
ifcana 1
ifcflag 1
ifcout 200
mustar 0.1
natifc 2
ng2qpt 16 16 16
ngqpt 4 4 4
nph11 1
nqpath 5
prt_ifc 1
prtdos 1
qpath 0.0 0.0 0.0
      0.0 0.0 1/8
      0.0 0.0 1/4
      0.0 0.0 1/2
      0.0 0.0 1
qph11 0.0 0.0 0.0 1
sydynmat 0
```

Supplementary Fig. 4. ANADDB (ABINIT utility) input automatically generated by Corvus from the Corvus input shown in Supp. Fig. 1. This information is used, together with the data generated by the input in Supp. Fig 2, to automatically create the dynamical matrix to be used in the next step. Other input files, such as the ANADDB “files” definition file, and the input file for the merging of the databases are not shown.

```
0
8
300 1.0 300.0
0
corvus.dym
1
2 1 0 3.0
2 2 0 3.0
```

Supplementary Fig. 5. DMDW input automatically generated by Corvus from the Corvus input shown in Supp. Fig. 1. This information is used, together with the dynamical matrix generated by the input in Supp. Fig 4 and stored in the `corvus.dym` file, to automatically calculate the Debye-Waller factors.