

```

1  int main() {
2  printf("hello, world");
3  return 0;
4  }

```

Code 1: Example from external file

```

1  &CONTROL
2  calculation      = 'scf',
3  outdir           = '/scratch1/christian.llemit/tmp/ZnO/Zn_i-p1/bands',
4  prefix          = 'Zn_i-p1',
5  pseudo_dir      = '/home/christian.llemit/pseudopotentials/GBRV',
6  tprnfor         = .true.,
7  tstress         = .true.,
8  verbosity       = 'high',
9  /
10
11 &SYSTEM
12 Hubbard_U(1)    = 7,
13 Hubbard_U(2)    = 15,
14 degauss        = 0.001,
15 ecutrho        = 720.0,
16 ecutwfc        = 90,
17 ibrav          = 0,
18 lda_plus_U     = .true.,
19 lda_plus_u_kind = 0,
20 nat            = 73,
21 nbnd           = 955,
22 ntyp           = 2,
23 occupations     = 'smearing',
24 smearing       = 'gauss',
25 tot_charge     = +1,
26 /
27
28 &ELECTRONS
29 conv_thr       = 1d-07,
30 mixing_beta    = 0.4d0,
31 /
32
33 ATOMIC_SPECIES

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34  O      15.9994   o_pbe_v1.2.uspp.F.UPF
35  Zn     65.39    zn_pbe_v1.uspp.F.UPF
36
37
38  CELL_PARAMETERS angstrom
39      9.8400836900000002   0.0001330800000000   0.0001262290000000
40     -4.9199289190000002   8.5219279720000003   -0.0002023880000000
41      0.0000715790000000  -0.0000367300000000   10.5887274460000000
42
43  ATOMIC_POSITIONS crystal
44  Zn      0.221911745800   0.111229691400  -0.012667771600
45  Zn      0.221022617000   0.112120860600   0.492073082100
46  Zn      0.218275460100   0.442221973100  -0.003589824100
47  Zn      0.221449396100   0.443831983000   0.491247851100
48  Zn      0.221927988300   0.776845208400  -0.012656918500
49  Zn      0.221044920200   0.775085343400   0.492071201200
50  Zn      0.556305426100   0.111217979300  -0.012659961700
51  Zn      0.558070464200   0.112104739800   0.492071733500
52  Zn      0.554571511400   0.442166315600  -0.004201058800
53  Zn      0.544937912400   0.422995822000   0.471789947100
54  Zn      0.554596752500   0.778557668200  -0.004228994400
55  Zn      0.545047255800   0.788143943400   0.471880323500
56  Zn      0.890931247300   0.114878951500  -0.003598004000
57  Zn      0.889341437700   0.111733105100   0.491243581900
58  Zn      0.890926799500   0.442225134200  -0.003568443100
59  Zn      0.889308476200   0.443855893300   0.491259045300
60  Zn      0.890974017500   0.778575869000  -0.004208862900
61  Zn      0.910134971900   0.788223087200   0.471815401200
62  Zn      0.111709527700   0.221457809900   0.242225907400
63  Zn      0.111101857100   0.222041345400   0.742634380600
64  Zn      0.111700036500   0.556457204400   0.242235778300
65  Zn      0.111100098700   0.555195346500   0.742645606200
66  Zn      0.116392112700   0.891290223600   0.233701818800
67  Zn      0.112051325700   0.889079744300   0.740393708300
68  Zn      0.441861010400   0.216752936700   0.233694385000
69  Zn      0.444049886100   0.221072991500   0.740396377200
70  Zn      0.443543093300   0.554881059300   0.240095692800
71  Zn      0.426568079800   0.546323670100   0.756304121200
72  Zn      0.441883057800   0.891274386000   0.233721153300
73  Zn      0.444068749200   0.889066064500   0.740386503900
74  Zn      0.776705029900   0.221464773700   0.242233069400
75  Zn      0.777947009600   0.222042604600   0.742642447400
76  Zn      0.778271660800   0.554894325900   0.240116282700
77  Zn      0.786788279800   0.546338325600   0.756342179300
78  Zn      0.778289893600   0.889632847800   0.240087907700

```

79	Zn	0.786808698800	0.906570010400	0.756289569000
80	Zn	0.666743213400	0.666349306500	0.597519542000
81	0	0.221260692300	0.111887159500	0.176178376400
82	0	0.222112325300	0.111016223700	0.680381712900
83	0	0.221792657200	0.443999619500	0.184493205000
84	0	0.219391632900	0.442762465600	0.680138896100
85	0	0.221281225700	0.775568476600	0.176188552100
86	0	0.222129316200	0.777215354100	0.680381970900
87	0	0.557590883100	0.111872382700	0.176185702600
88	0	0.555922683900	0.111003919900	0.680381914200
89	0	0.555093869000	0.443232528900	0.185258709100
90	0	0.559432536600	0.451844919900	0.679041975200
91	0	0.555117245100	0.778045504300	0.185224916600
92	0	0.559471931600	0.773665422000	0.679019554500
93	0	0.889167664200	0.111379415400	0.184485394600
94	0	0.890380769400	0.113752876700	0.680135407500
95	0	0.889150206300	0.444012301900	0.184513634100
96	0	0.890375802300	0.442766033900	0.680148016500
97	0	0.889917214100	0.778062382500	0.185249266700
98	0	0.881270627900	0.773693902700	0.679035805800
99	0	0.111138383100	0.222036472600	0.431631645300
100	0	0.110449988500	0.222707394300	0.930778396900
101	0	0.111103643900	0.555285086500	0.431639728500
102	0	0.110438053900	0.553906760400	0.930790205100
103	0	0.123556692000	0.894861206200	0.424387453000
104	0	0.109413198900	0.887780992900	0.928212041400
105	0	0.438280121500	0.209575057800	0.424381749400
106	0	0.445363717800	0.223729637900	0.928215586300
107	0	0.448524373700	0.557356662800	0.434527748400
108	0	0.443357685200	0.554751711400	0.939040973700
109	0	0.438314739000	0.894836169300	0.424402351700
110	0	0.445370076700	0.887776392600	0.928202605700
111	0	0.777870624000	0.222061648800	0.431637505600
112	0	0.779244097400	0.222716024500	0.930786885100
113	0	0.775754408100	0.557403023700	0.434568563100
114	0	0.778379048600	0.554766464900	0.939067243100
115	0	0.775818344100	0.884668218600	0.434512210900
116	0	0.778399548700	0.889799320600	0.939030963300
117				
118	K_POINTS automatic			
119	3	3	3	0 0 0