

## Code 1: Hello World

```

1 &CONTROL
2   calculation      = 'scf',
3   outdir           =
4   ↪ '/scratch1/christian.llemit/tmp/ZnO/Zn_i-p1/bands',
5   prefix           = 'Zn_i-p1',
6   pseudo_dir       =
7   ↪ '/home/christian.llemit/pseudopotentials/GBRV',
8   tprnfor          = .true.,
9   tstress          = .true.,
10  verbosity        = 'high',
11 /
12 &SYSTEM
13   Hubbard_U(1)     = 7,
14   Hubbard_U(2)     = 15,
15   degauss          = 0.001,
16   ecutrho          = 720.0,
17   ecutwfc          = 90,
18   ibrav            = 0,
19   lda_plus_U       = .true.,
20   lda_plus_u_kind  = 0,
21   nat              = 73,
22   nbnd             = 955,
23   ntyp             = 2,
24   occupations      = 'smearing',
25   smearing         = 'gauss',
26   tot_charge       = +1,
27 /
28 &ELECTRONS
29   conv_thr         = 1d-07,
30   mixing_beta      = 0.4d0,
31 /
32 ATOMIC_SPECIES
33   O      15.9994   o_pbe_v1.2.uspp.F.UPF
34   Zn     65.39    zn_pbe_v1.uspp.F.UPF
35
36
37 CELL_PARAMETERS angstrom
38   9.8400836900   0.0001330800   0.00012622900
39

```

```

40 -4.9199289190   8.52192797200  -0.00020238800
41   0.0000715790  -0.0000367300   10.58872744600
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   O       0.221260692300   0.111887159500   0.176178376400
82   O       0.222112325300   0.111016223700   0.680381712900
83   O       0.221792657200   0.443999619500   0.184493205000
84   O       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

```

Code 2: Hello World

```

1 &CONTROL
2 calculation = 'vc-relax',
3 etot_conv_thr = 1.d-5,
4 forc_conv_thr = 1.d-4,
5 outdir =
↳ '/scratch1/christian.llemit/tmp/Zn0/relax/Zn_vac-n2',

```

```

6 prefix = 'Zn_vac-n2',
7 pseudo_dir = '/home/christian.llemit/pseudopotentials/GBRV',
8 tprnfor = .true.,
9 tstress = .true.,
10 verbosity = 'high',
11 /
12
13 &SYSTEM
14 celldm(1) = 18.61865901,
15 degauss = 0.01,
16 ecutrho = 720.0,
17 ecutwfc = 90,
18 ibrav = 0,
19 nat = 71,
20 ntyp = 2,
21 occupations = 'smearing',
22 smearing = 'gauss',
23 tot_charge = -2,
24 /
25
26 &ELECTRONS
27 conv_thr = 1.00000e-06,
28 mixing_beta = 7.00000e-01,
29 /
30
31 &IONS
32 /
33
34 &CELL
35 /
36
37 ATOMIC_SPECIES
38 Zn 65.39 zn_pbe_v1.uspp.F.UPF
39 O 15.9994 o_pbe_v1.2.uspp.F.UPF
40
41
42 CELL_PARAMETERS alat
43 0.9992341179999999 0.0000032780000000 -0.0000021060000000
44 -0.4996142200000000 0.8653637700000000 0.0000021060000000
45 -0.0000022630000000 0.0000013060000000 1.0762002420000001
46
47 ATOMIC_POSITIONS crystal
48 Zn 0.225724334000 0.114469544000 0.491450723000
49 Zn 0.111704132000 0.222521937000 0.241987109000

```

50	O	0.221485939000	0.110948003000	0.180189772000
51	O	0.110322337000	0.221831003000	0.431825913000
52	Zn	0.222194323000	0.110873993000	0.991530280000
53	Zn	0.111630968000	0.222483807000	0.741620488000
54	O	0.221473888000	0.110568370000	0.681197816000
55	O	0.110750331000	0.222042093000	0.930996932000
56	Zn	0.225735420000	0.444605150000	0.491445304000
57	Zn	0.110604765000	0.554533468000	0.243231178000
58	O	0.221485737000	0.443871409000	0.180188013000
59	O	0.110456814000	0.554251379000	0.432423130000
60	Zn	0.222195830000	0.444655023000	0.991530030000
61	Zn	0.111325965000	0.555980387000	0.741094871000
62	O	0.221473355000	0.444238883000	0.681196210000
63	O	0.111388717000	0.556109046000	0.930719707000
64	Zn	0.222226193000	0.777773807000	0.489436477000
65	Zn	0.110602814000	0.889397186000	0.243228014000
66	O	0.222224168000	0.777775832000	0.182605934000
67	O	0.110458475000	0.889541525000	0.432424563000
68	Zn	0.222225582000	0.777774418000	0.992901807000
69	Zn	0.111325600000	0.888674400000	0.741096833000
70	O	0.222223945000	0.777776055000	0.679955230000
71	O	0.111389522000	0.888610478000	0.930721053000
72	Zn	0.555406396000	0.114461929000	0.491451180000
73	Zn	0.446011020000	0.225358036000	0.243518273000
74	O	0.556128831000	0.110947502000	0.180190445000
75	O	0.433589789000	0.200513843000	0.424119728000
76	Zn	0.555347233000	0.110870398000	0.991531865000
77	Zn	0.445373083000	0.224080234000	0.738636233000
78	O	0.555762155000	0.110568197000	0.681198094000
79	O	0.443016927000	0.219364979000	0.931407379000
80	Zn	0.446006031000	0.553993969000	0.243530794000
81	O	0.555552891000	0.444447109000	0.176450783000
82	O	0.433585923000	0.566414077000	0.424117600000
83	Zn	0.555553130000	0.444446870000	0.985217120000
84	Zn	0.445371021000	0.554628979000	0.738630029000
85	O	0.555553941000	0.444446059000	0.702884490000

86	O	0.443014501000	0.556985499000	0.931403488000
87	Zn	0.555394850000	0.774264580000	0.491445304000
88	Zn	0.445466532000	0.889395235000	0.243231178000
89	O	0.556128591000	0.778514263000	0.180188013000
90	O	0.445748621000	0.889543186000	0.432423130000
91	Zn	0.555344977000	0.777804170000	0.991530030000
92	Zn	0.444019613000	0.888674035000	0.741094871000
93	O	0.555761117000	0.778526645000	0.681196210000
94	O	0.443890954000	0.888611283000	0.930719707000
95	Zn	0.888887602000	0.111112398000	0.492361738000
96	Zn	0.777484497000	0.222515503000	0.241984281000
97	O	0.888889591000	0.111110409000	0.181750148000
98	O	0.778171989000	0.221828011000	0.431825379000
99	Zn	0.888889985000	0.111110015000	0.992266090000
100	Zn	0.777520237000	0.222479763000	0.741623020000
101	O	0.888889311000	0.111110689000	0.681763702000
102	O	0.777959329000	0.222040671000	0.930997750000
103	Zn	0.885538071000	0.444593604000	0.491451180000
104	Zn	0.774641964000	0.553988980000	0.243518273000
105	O	0.889052498000	0.443871169000	0.180190445000
106	O	0.799486157000	0.566410211000	0.424119728000
107	Zn	0.889129602000	0.444652767000	0.991531865000
108	Zn	0.775919766000	0.554626917000	0.738636233000
109	O	0.889431803000	0.444237845000	0.681198094000
110	O	0.780635021000	0.556983073000	0.931407379000
111	Zn	0.885530456000	0.774275666000	0.491450723000
112	Zn	0.777478063000	0.888295868000	0.241987109000
113	O	0.889051997000	0.778514061000	0.180189772000
114	O	0.778168997000	0.889677663000	0.431825913000
115	Zn	0.889126007000	0.777805677000	0.991530280000
116	Zn	0.777516193000	0.888369032000	0.741620488000
117	O	0.889431630000	0.778526112000	0.681197816000
118	O	0.777957907000	0.889249669000	0.930996932000
119				
120	K_POINTS automatic			
121	2	2	2	0 0 0