materials

MDPI

Supplementary

Electronic Transport Properties of Silicane Determined from First Principles

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We provide the input files used for the Quantum espresso self-consistent runs (scf.in), the phonon calculations (ph.in), the input for the transformation of the force constants to real space (q2r.in), the input file for the non-selfconsistent run (nscf.in), and the input file for the electron-phonon Wannier (EPW) code.

Self-consistent calculations file (scf.in):

```
&CONTROL
   calculation = 'scf' ,
   prefix = 'Silicane' ,
   wf_collect = .true.
   outdir = './' ,
   pseudo_dir = './' ,
   etot_conv_thr = 1.0d-6 ,
/
&SYSTEM
   ibrav = 0,
   a = 3.88717,
   nat = 4,
   ntyp = 2,
   ecutwfc = 50.0,
 /
&ELECTRONS
   conv_thr = 1.0d-12 ,
   mixing_beta = 0.7 ,
 /
 &IONS
 /
 &CELL
 /
CELL_PARAMETERS alat
       0.500000000       0.866025404       0.000000000
      −0.500000000       0.866025404       0.000000000
       0.000000000       0.000000000       5.144000000
ATOMIC_SPECIES
    Si     28.08550    Si.upf
```

```
   H          1.008       H.upf
ATOMIC_POSITIONS crystal
   H          0.000000000       0.000000000       0.000000000
   Si         0.000000000       0.000000000       0.075118000
   Si         0.333333333       0.333333333       0.111100000
   H          0.333333333       0.333333333       0.186218000
K_POINTS automatic
24 24 1 0 0 0
```