Unix shell-script

```sh
#!/bin/sh

rm -f si.etot_vs_ecut.dat

for ecut in 12 16 20 24 28 32
do
    cat > pw.si.scf.$ecut.in << EOF
 &CONTROL
    prefix='silicon',
 /
 &SYSTEM
    ibrav =  2,
    celldm(1) = 10.2,
    nat =  2,
    ntyp = 1,
    ecutwfc = $ecut,
 /
 &ELECTRONS
 /
ATOMIC_SPECIES
   Si  28.086  Si.pz-vbc.UPF
ATOMIC_POSITIONS
   Si 0.00 0.00 0.00
   Si 0.25 0.25 0.25
K_POINTS automatic
   4 4 4    1 1 1
EOF

    pw.x -in pw.si.scf.$ecut.in > pw.si.scf.$ecut.out

    grep -e 'kinetic-energy cutoff' -e ! pw.si.scf.$ecut.out | \
        awk '/kinetic-energy/ {ecut=$(NF-1)}
             /!/              {print ecut, $(NF-1)}' >> si.etot_vs_ecut.dat

done
```

PWTK script

```
load_fromPWI ../pw.si.scf.in

set fid [open si.etot_vs_ecut.dat w]

foreach ecut {12 16 20 24 28 32} {
    SYSTEM "ecutwfc = $ecut"
    runPW pw.Si.scf.$ecut.in

    puts $fid "$ecut [::pwtk::pwo::totene pw.Si.scf.$ecut.out]"
}
close $fid
```