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# Challenges and clarification on creating input files for metallic materials in the noncollinear spin-orbit case and band structure within GGA in Quantum Espresso: Ni as a case study

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**Abstract.** We have explicitly illustrated the challenges faced in creating input files for metallic materials in Quantum espresso by calculating the band structure of Ni and clarifying with the flags provided in this work. In this paper, we calculated the band structure of Ni after optimizations of the lattice constant, kinetic energy cutoff, ecutrho, k-points and described the basic parameters required for metallic materials. The input files provided in our work have been set such that the problem of spin/noncolin parameters and challenges faced by researchers trying to find the band structure of metallic materials have been solved. Some of these are presence of smearing, tprnfor, default nbnd, lspinorb, e.t.c.

**Keywords:** Noncollinear, nspin, Band Structure, tprnfor, metallic

## 1.0. Introduction

There are only four elements that are magnetic at room temperature or close to room temperature of which nickel is one (cobalt, iron, gadolinium and nickel)[1]. Nickel is a magnetic material that also shows half-magnetic properties[2]. It has Face Centered Cubic (FCC) crystal structure[3,4] with the atomic mass 58.6934a.m.u[5].

Investigating the electronic structure of metals has been a major challenge since decades, especially transition metals. Different researchers have done their investigations and came up with varying results[6]. The major key to this variation is the lack of proper care needed, noting that the pseudopotentials used have great impact on the calculations. However, reasonable closely related results may be obtained taking into account different pseudopotentials.

For instance, band structure of Iron (Fe) has been investigated by Stern[7] and Wood[8] where their results were seen to have agreed comparing the 3d-bands character and wave function character for their different calculations (different choice of pseudopotentials).

## 2.0. Computational details

Preceding the electronic structure calculation were the optimizations including the lattice constant, k-points, kinetic energy cutoff and ecutrho emerging at 6.532964368 Bohr, 10x10x10 Monkhorst-



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Pack[9] k grids being the commonly used these days[10] at gamma point, 80 Ry cutoff energy and 510 Ry ecutrho respectively. Consistency with these values was not overemphasized throughout our calculations[11]. In the overall input parameters, same parameters were used for the variable cell relaxation, self consistency, non-self consistency and bands calculation with the basic difference vc-relax, scf, nscf and bands which depict what type of calculation is run. In the bands calculation, we explicitly stated the k path[9,12]. The vc-relax, scf, nscf and bands calculations will run under pw.x, the post-processing of bands run under bands.x and the plotband run under plotband.x completing the whole cycle of the band structure.

The Quantum espresso package[13–16] has been used to carry out our calculations within the GGA[17] approximations based on density functional theory (DFT)[18–20], being one of the most useful packages in estimating the electronic properties (band structure) of materials[2].

During our computation, some of the challenges faced by researchers trying to investigate the electronic properties of magnetic materials were put to test causing the calculation to; not converge, display properties different from that of metals, truncate the nscf calculation (e.g internal error, cannot bracket Ef) and so on. These errors and challenges have been corrected with the appropriate flags described below. An example is the use of smearing in the occupations where the occupations = 'smearing', smearing type can be optional and the degauss must be included[2]. This has been studied for metals which distinguishes them from other insulating materials or semiconductors.

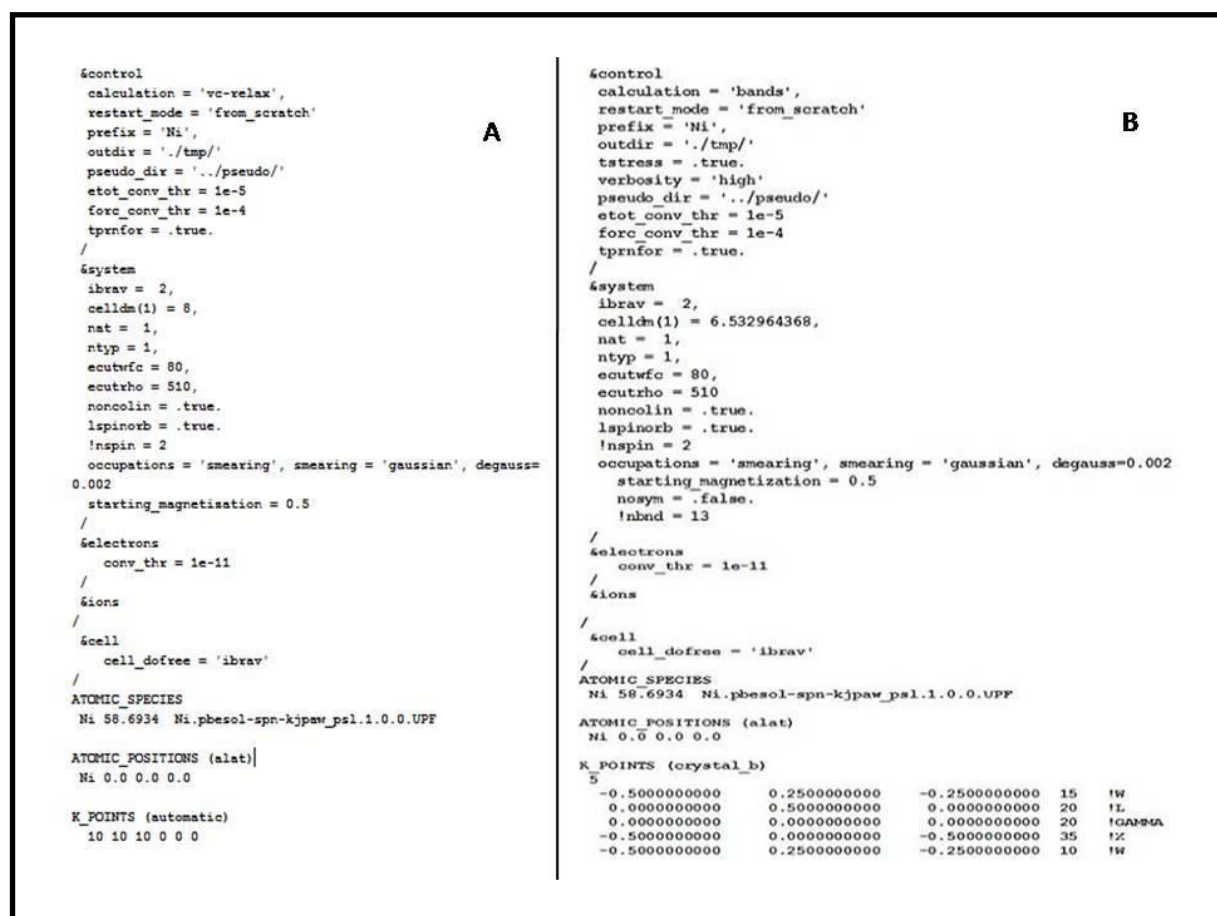


Figure 1: 'A' input file for vc-relax of Ni and 'B' input file for the bands calculation.

<b>&amp;Bands</b> <b>prefix = 'Ni'</b> <b>filband = 'Ni.bands.dat'</b> <b>outdir = './tmp/'</b> <b>/</b>	<b>C</b>	<b>Ni.bands.dat</b> <b>-5 48</b> <b>bands.xmgr</b> <b>bands.ps</b> <b>19.0449</b> <b>4.00 19.0449</b>	<b>D</b>
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Figure 2: 'C' shows the post-processing file making the bands' result from 'B' readable and 'D' is the plotband input file.

### 2.1. Flags and their meaning

- Calculation: This is the type of calculation such as vc-relax, scf, nscf, bands e.t.c
- Restart\_mode; here, 'from\_scratch' is the default mode to carry out plane-wave calculation
- Prefix: is the input filename chosen by the user and must remain same throughout the calculation
- Verbosity = 'high', 'debug' and 'medium' work same way
- Outdir: This is where the temporary files not needed after the calculations are stored. This would be created automatically if not present
- Pseudo\_dir is a directory for pseudopotential files
- etot and forc\_conv\_thr are normal settings for vc-relax
- tprnfor calculates the forces when set true
- ibrav is the bravais lattice equals 0 when providing crystal axis in the input, 1 for simple cubic, 2 for face centered cubic, 3 for base centered cubic, 4 for hexagonal and trigonal P and so on[21]
- celldm is the lattice constant or lattice parameter. It is from celldm(1) to celldm(6) in Bohr or A, B, C, CosAB, CosAC, CosBC in Angstrom. Here, celldm(1) indicates the length 'a' in Bohr.
- noncolin set the calculation to be noncollinear when true. We have set the nspin as default in our calculation since setting the noncolin and nspin true simultaneously contradicts each other. This implies that noncolin should be false when the spin orientation is considered and vice versa.
- lspinorb makes the noncollinear code use spin-orbit pseudopotential when set true
- nat is the total number of atoms (1 Ni atom)
- ntyp is the number of different type of atoms (here 1, just Ni)
- ecutwfc is the kinetic energy cutoff which makes the result more accurate (higher values)
- ecutrho is the kinetic energy cutoff for charge density and potential (in Ry)
- conv\_thr is the electrons' convergence threshold (better at lower values)
- ions tells the movement of the atoms
- cell is related to the movement of the unit cell, meaning that "ibrav" is the parameter that should be relaxed/unchanged here. Some other parts of the structure could also be relaxed when defined here depending on the need (cell\_dofree)
- Ni.pbesol-spn-kjpaw\_psl.1.0.0.UPF is the pseudopotential which must be in the pseudo directory specified above
- Atomic\_Positions displays the coordinates of the atoms in the unit cell, can be in alat in Cartesian axis[9,12]angstrom, bohr e.t.c.
- nbnd is number of bands (valence bands). About half of the total bands would be used if not stated (exactly half for insulators and semiconductors, a little more than half for metals)
- Occupations such as smearing (metals), tetrahedra[10] which is more appropriate for nscf and DOS calculation for nonmetals
- smearing:- gaussian is the default but can always be changed to suit your calculation
- degauss is the value of the gaussian spreading (for metals)

- nspin:- the noncolin and nspin are conflicting flags, both should not be present within the same calculation
- starting\_magnetization of your choice is required
- k-points; more k-points are needed for calculations like nscf, meanwhile gamma point can be used for isolated calculation. It is more convenient to use 'alat' in crystals stating the positions of each atom. "crystal\_b" or 'tpipa\_b' are used when explicitly stating the k\_paths as in case of the bands calculation[21]. In nscf calculation, depending upon the system, the k-point mesh should be made at least twice the k-point mesh used for the scf calculation.
- filband; the file containing data of the band (output file of the bands)

### 3.0. Results and discussion

#### 3.1 Band Structure

The bands of solids are theoretically infinite similar to that of atoms. Also, the widths of bands vary depending on the properties of the atomic orbital which they originate[2]. The Fermi energy of Ni was observed to be 19.0449 eV when the energy band was plotted along high symmetry points W, L, GAMMA, X and W in the Brillouin zone. The optimized lattice constant was used consistently to study the electronic band structure of Ni within the GGA approximation. Unarguably, the lattice constant is overestimated[22] and band gap is underestimated[22,23] for semiconductors and insulators within GGA approximation, but the case is quite different for metals[24,25] since there is no clear band gap for metals. Comparison of our band structure with[2,26,27] shows a very good agreement. Ni is found to have a direct band gap with the conduction band minimum between Gamma and X, while the valence band maximum is found at Gamma point[2].

Table 1: The lattice constant of Ni.

	This work	Other works
Lattice constant (Bohr)	6.53296	6.30504[6], 6.61311[28]

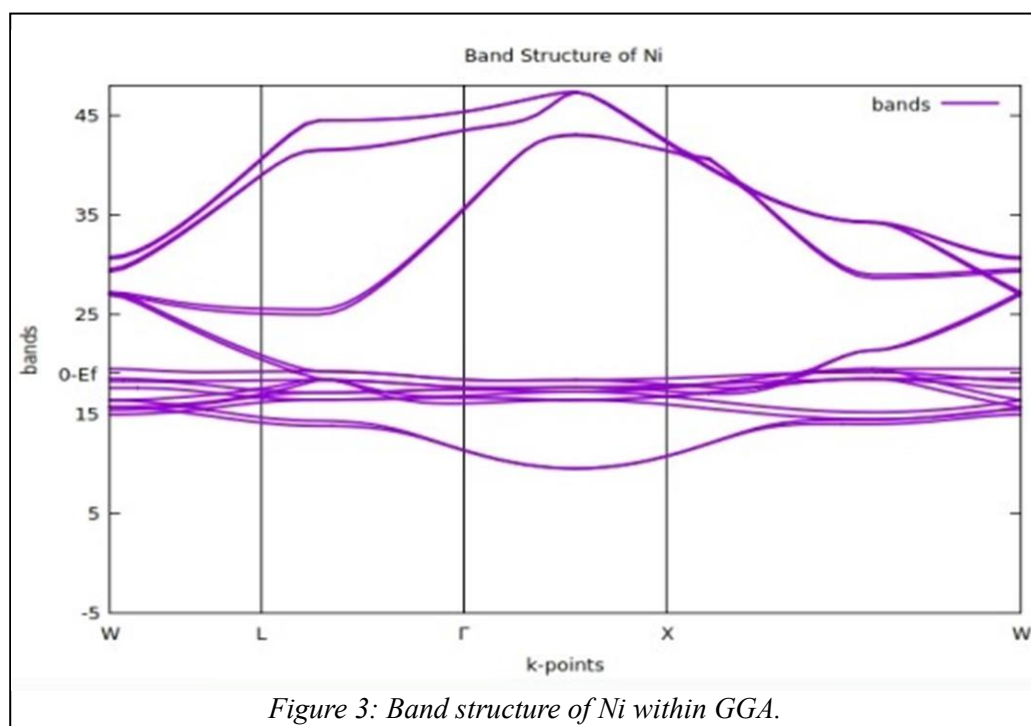


Figure 3: Band structure of Ni within GGA.

#### 4.0. Conclusion

In order to make the write-up concise as possible, researchers can also try setting each of the input parameters of various flags to default or playing around their modes to detect what difference it would make to their calculations (if any), noting that only the very essential points have been detailed here in this paper.

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We would like to acknowledge Professor Ranjan Kumar and Dr. Shahid Sattar for their undaunted support every now and then. The simulations described in this work were carried out on King AbdulAziz University's high performance computing resource (AZIZ Supercomputer) (<http://hpc.kau.edu.sa>).

#### Conflict of Interest

The authors declare no conflict of interest.

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