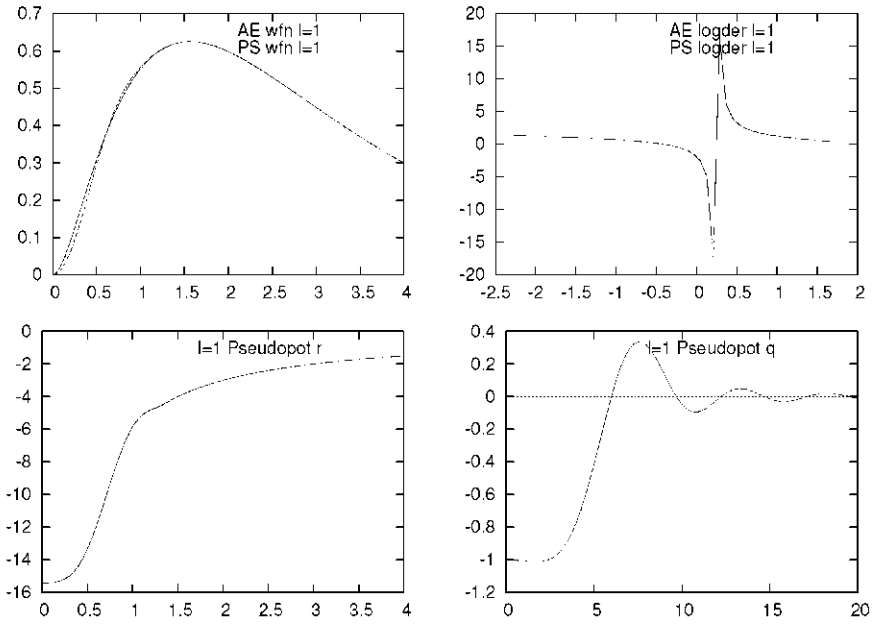

Figure 5.5: Boron p type orbitals: (top left) all electron wavefunction and pseudowavefunction; (top right) the logarithmic derivative of the wavefunctions - shows the discontinuity at r_c; (bottom left) the pseudopotential; (bottom right) the Fourier transform of the pseudopotential

For nitrogen, the $1s$ orbital is again included in the ionic core, the $2p$ orbital is populated with two electrons and the $2p$ orbital is populated with three electrons; for all orbitals the cutting radius r_c was chosen 1.45 Bohrs.

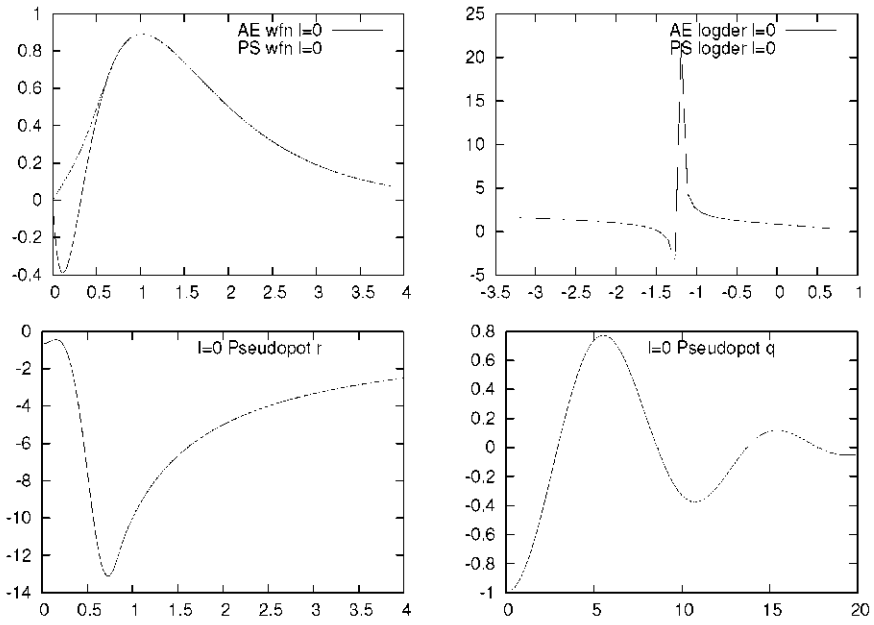

Figure 5.6: Nitrogen s type orbitals: (top left) all electron wavefunction and pseudowavefunction; (top right) the logarithmic derivative of the wavefunctions - shows the discontinuity at r_c; (bottom left) the pseudopotential; (bottom right) the Fourier transform of the pseudopotential

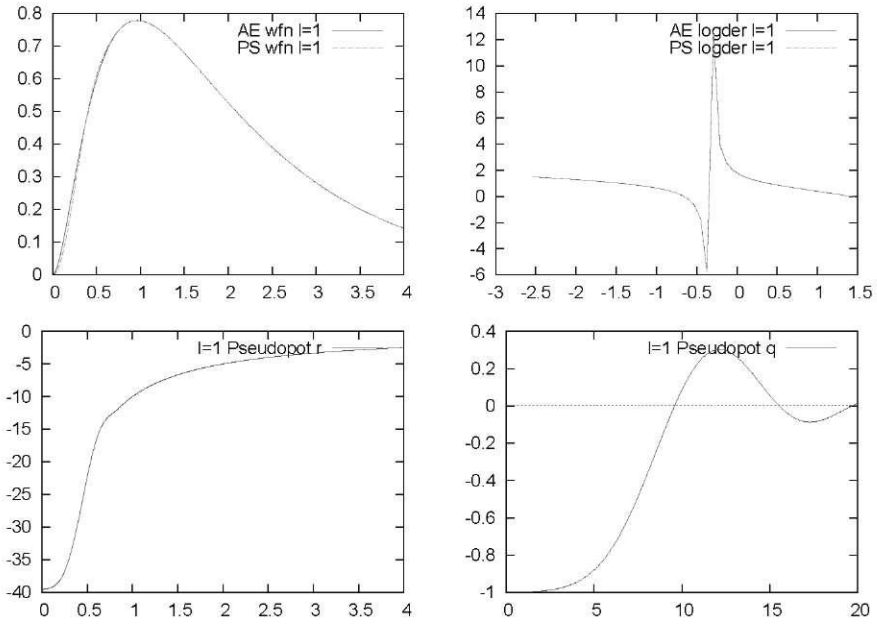

Figure 5.7: Nitrogen p type orbitals: (top left) all electron wavefunction and pseudowavefunction; (top right) the logarithmic derivative of the wavefunctions - shows the discontinuity at r_c; (bottom left) the pseudopotential; (bottom right) the Fourier transform of the pseudopotential

5.3 Band structure DOS for bulk BN

Boron nitride (BN) is a wide band-gap semiconductor (5.05 eV - amorphous, 5.2 eV - hexagonal, 4.5-5.5 eV würtzite, 5.5 eV - diamond) [29] [30]. BN is not found in nature and amorphous-BN is produced synthetically from boric acid or boron trioxide. Alternate methods of preparation or subsequent treatment is required in order convert the amorphous form into others; for example, hexagonal BN is obtained by reacting boron trioxide or boric acid with ammonia or urea in a nitrogen atmosphere, and würtzite BN is obtained by high-pressure or by dynamic shock methods.

It must be mentioned that only graphene-like BN nanotubes have been synthesized and that no records of würtzite BN nanowires or nanotubes currently exist.

For the confirmation of the pseudopotentials' transferability, the energy dispersion and density of states (DOS) have been plotted out for the bulk material (Fig.5.8) of würtzite structure (Fig.5.9). The band structure is in agreement with that obtained by other *ab initio* calculations [28] and the bandgap value is also close to those measured experimentally: 5.9 eV, obtained here, as compared to the measured values of 5.5 eV [29] [30].

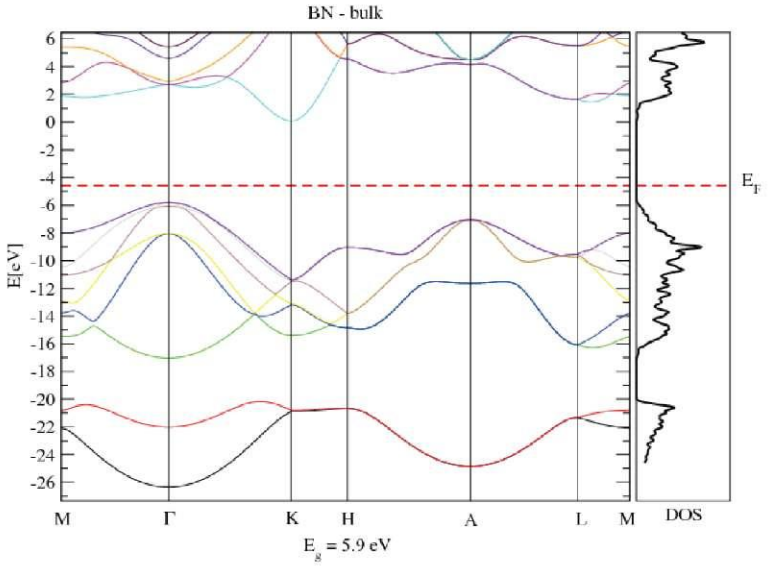

Figure 5.8: Band structure and density of states for bulk BN

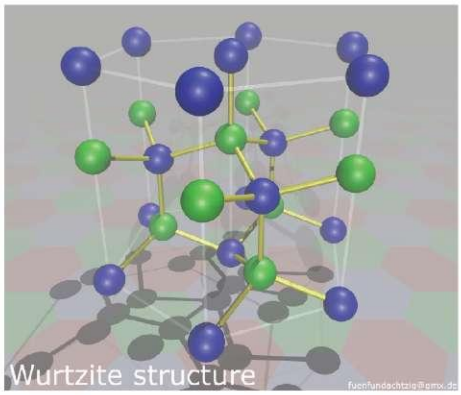

Figure 5.9: Atomic structure of würtzite BN crystal

Because for the q-1D structures the periodicity is maintained only in the Γ-A direction and in order to easily detect the differences in band structure between the bulk material and the q-1D structures, the energy dispersion relation was mapped out for the Γ-A direction in the bulk material (see Fig. 5.10). It must be specified that the DOS corresponding to the conduction band appears to be overhanging beyond the last represented state, but that is the contribution from k-states that are not visible in the Γ-A representation but that can be seen in the vicinity of the K point (Fig.5.8).

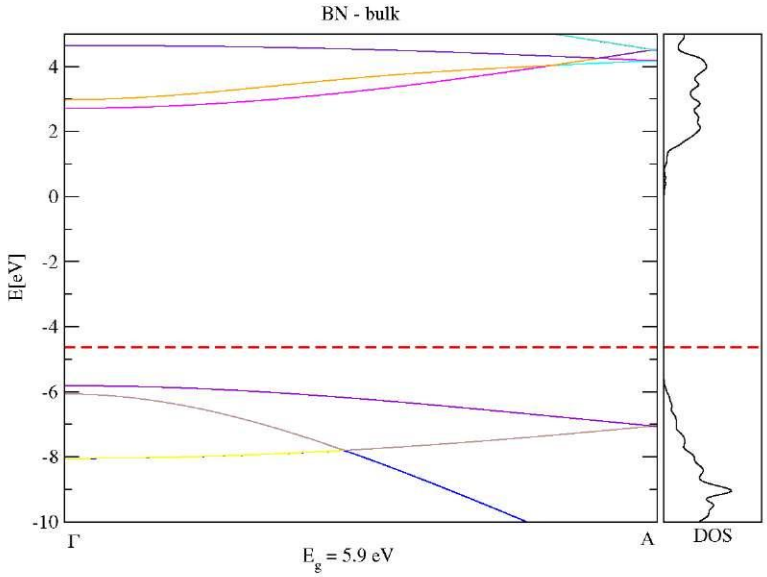

Figure 5.10: Band structure and density of states for bulk BN between Γ and A points

5.4 Band structure, DOS and plotted wavefuntions for the q-1D structures

In order to associate the data to the corresponding structure in a more straightforward manner and in order to avoid repeating the representations of the unrelaxed and relaxed nanowires/nanotubes in a separate section of this chapter, images with sections of the nanotubes and nanowires, both before and after relaxation, are placed next to the graphs.

For all band structure and DOS investigations the structural relaxation was carried out in multiple steps in order to ensure the accuracy of the final results; this is done by comparing the band structures for two successive relaxation steps until no important changes arise.

As a general notation, 'R' stands for the outer radius and 'r' stands for the internal radius of the tube.

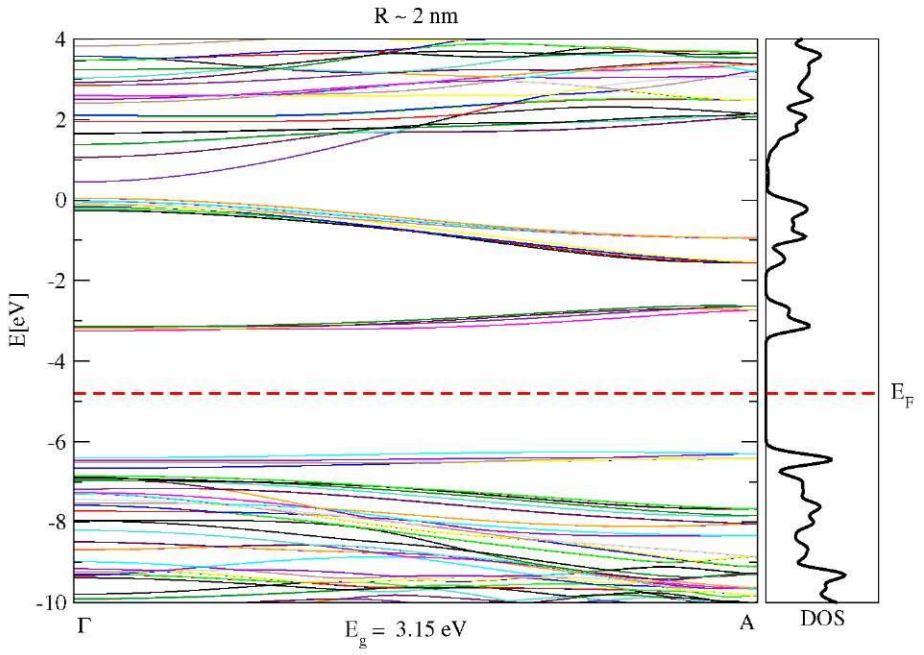

Figure 5.11: Band structure and DOS for the nanowire with R = 2 nm, r = 0 nm

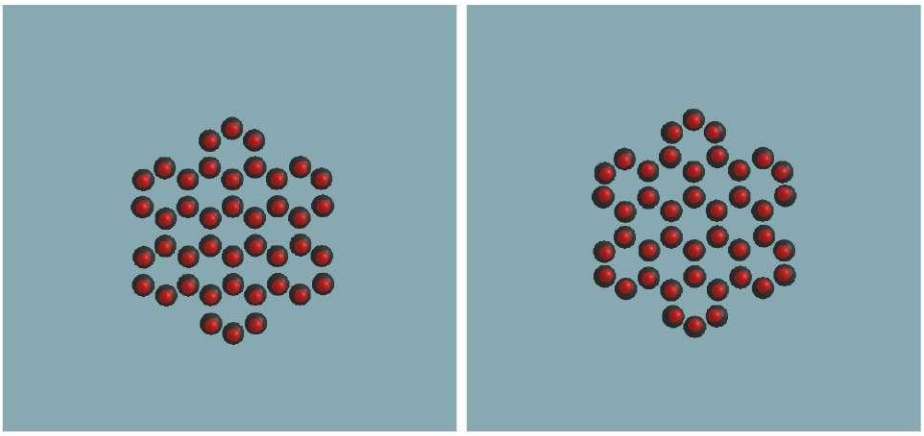

Figure 5.12: Input positions and relaxed, output positions for the nanowire with R = 2 nm (boron in red and nitrogen in blue)