Modifications in generlcgo.F90

Some modifications in generlcgo.F90 are crucial for mixed systems. The example used here is NaH_2O. When init_lcao is set to 1, the initialization of the wave functions is done by calling the subroutine genermowf in generlcgo.F90. The spin assigment is first done in the subroutine iniqnb (in init.F90), giving spins up first and then spins down. Then an other (thus different) assignment is done again in the subroutine genermowf called later on, which was in the previous version as followed:

```
DO ion=1,nion
  DO natlevel=1,nmaxst(ion)
    numstate = 1 + numstate
#if(fullspin)
    nactst(ion) = nactst(ion)+MOD(natlevel,2)
    ispin(numstate) = 2-MOD(natlevel,2)
#else
    nactst(ion) = nactst(ion)+1
#endif
(...)
  ENDDO
ENDDO
```

This means for NaH_2O:

- Na: numstate=1, ispin=1
- O: numstate=2, ispin=1
  numstate=3, ispin=2
  numstate=4, ispin=1
  numstate=5, ispin=2
  numstate=6, ispin=1
  numstate=7, ispin=2
- H: numstate=8, ispin=1
- H: numstate=9, ispin=1

However there should be 4 spins down, and not 3. This means that the created system has a non-desired spin polarization. The solution is to set ispin(9) to 2. We then definitely need the ipol array. This table is defined in params.F90, initialized in initions (meaning that a last column has to be added in the for005ion input file), and used in genermowf as followed:

```
DO ion=1,nion
  DO natlevel=1,nmaxst(ion)
    numstate = 1 + numstate
#if(fullspin)
    nactst(ion) = nactst(ion)+MOD(natlevel,2)
    ispin(numstate) = 2-MOD(natlevel,2)
    IF (ipol(ion).eq.-1) THEN
       ispin(numstate) = 2-MOD(ispin(numstate)+1,2)
    ENDIF
#else
    nactst(ion) = nactst(ion)+1
#endif
(...)
  ENDDO
ENDDO
```