# How to make doping?

The 1st principle calculations are performed under the charge neutrality.

We have two method (or combined ) to treat fractional number of electrons in the primitive cell.

1. You can use fractional numbers for SPEC_ATOM_Z,
2. Set valence charge by BZ_ZBAK.

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Following sample is doping for Si, Z=14 and two atoms per cell.

## Fractional Z

, such as Z=14.2
Together with Z, you have to add SPEC_ATOM_Q= for atoms.
For example, for Z=14.2, we may need to add Q=2,2.2 (Note Q= is the initial valence electron density for {s} {p} {d} {f}, successively.)
Thus Q=2,2.2 implies adding +0.2 electron for p channel to keep charge neutrality of the
atom when we calculate spherical atomic densities.
Run lmfa with 'grep conf'.
It shows electron distribution of initial condition.
Then Q=0 (check of charge neutrality) is shown in the output of lmfa.
Pay attention that lmfa finishs normally.

Run lmf to keep the console output to llmf. Then

```
grep 'z=',llmf
```

shows Z for atoms.

PROF

```
grep -A5 'Charges:'
```

shows

```
Charges:  valence     8.40000   cores    20.00000   nucleii   -28.40000
   hom background     0.00000   deviation from neutrality:     -0.00000
```

Here we see nuclei = - 2* 14.2 = -28.4 # given by Z

CAUTION: at the first iteration, Charges: shows such as

```
  Charges:  valence     8.00000   cores    20.00000   nucleii
-28.00000
  hom background     0.12300   deviation from neutrality: 0.12300
```

because of the initial condition is given by superposition of atomic densities.
Deviation is nonzero ==> But 'deviation from neutrality: 0' from the next iteration.

## Back ground charge by ZBAK

Set BZ_ZBAK. If ZBAK=0.4, the back ground charge is negative as -0.4|e|,
thus the number of electron becomes 0.4 smaller.
(cores + valence electron + ZBAK = |total nucleus charge|).

```
 grep -A5 'Charges:'
```

shows

```
Charges:  valence     7.60000   cores    20.00000   nucleii   -28.00000
    hom background     0.40000   deviation from neutrality:     -0.00000
```

That is, 7.6+0.4+20.0 = -28.0

## Combination of fractional Z and BZ_ZBAK

Let us try Z=14.2, Q=2,2.2, together with ZBAK=0.3
In this case, we have

PROF

```
   Charges:  valence     8.10000   cores    20.00000   nucleii
-28.40000
    hom background     0.30000   deviation from neutrality:     -0.00000
```

This means that (2 atoms per cell).
nuclei = - 2* 14.2 = -28.4 # given by Z
cores = 2* 10 = 20 # given by the atom of integer part of Z.
background = 0.3 # given by ZBAK
Thus we have
valence electron = 28.4 - 20- 0.3 = 8.1