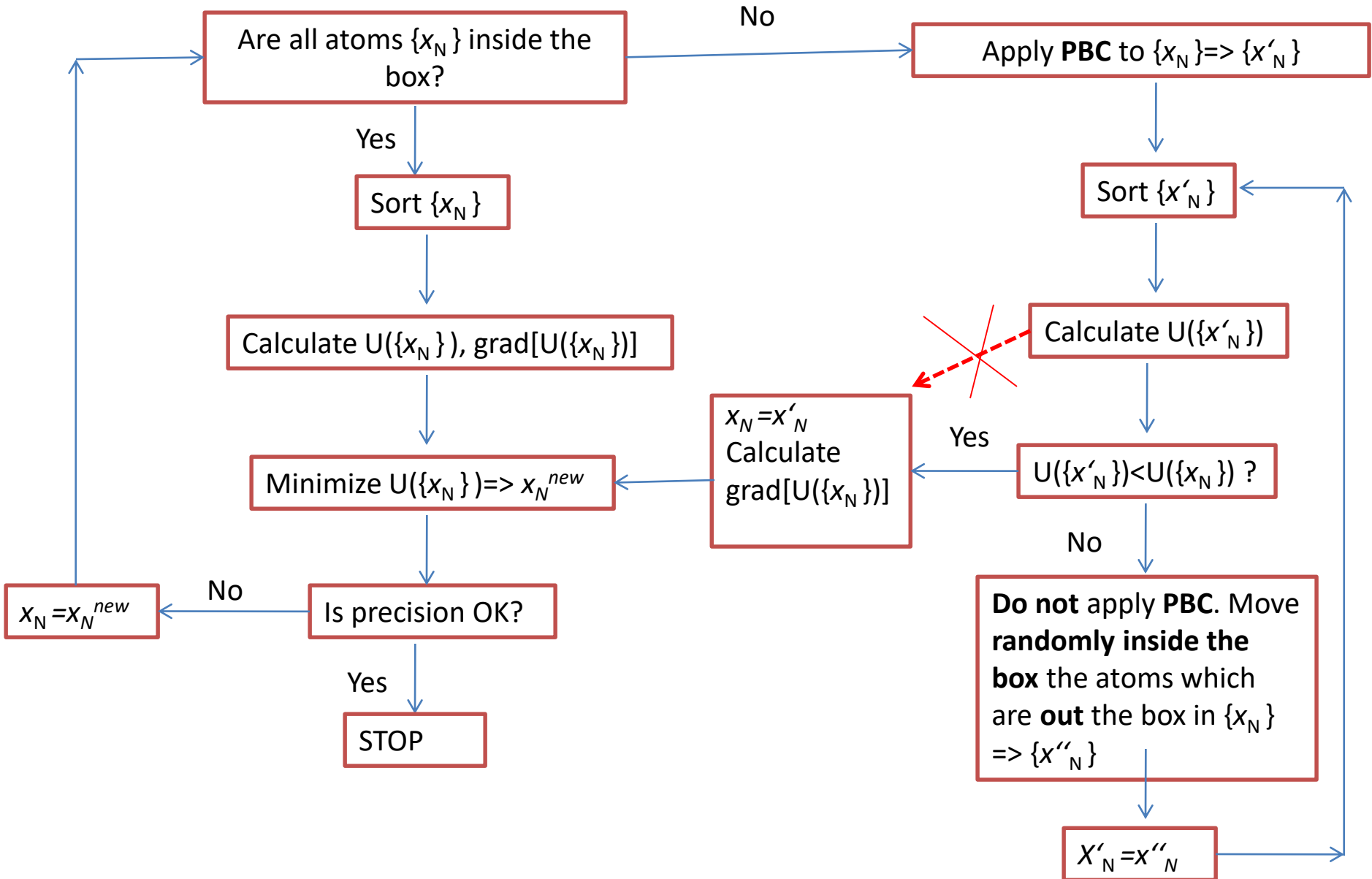
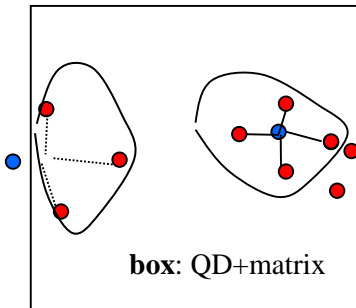
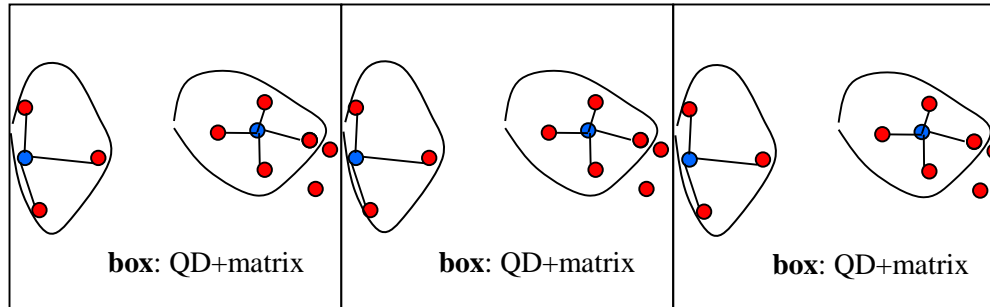


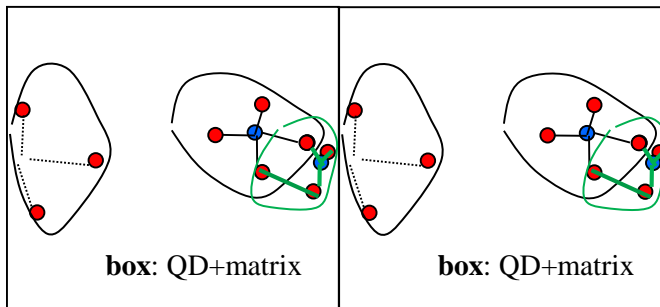
## Periodic boundary conditions (PBC) algorithm



Legend: ● Ga, ● As



Configuration in the next step: A **Ga** atom is taken out of the box.



Translation of **Ga** atom required by periodic boundaries

Translation of the **Ga** atom changes the energy of the configuration box breaks the symmetry of the atoms in the **box**: 3 bonds are broken and other 4 bonds appears by translation. Such a translation would't put back in the sum on the neighbor atoms from  $U$  the same energy as before the translation.

## Symmetry breaking in crystal by PBC translation

