**Hands on 7**

**Bhuvanesh P – MM19B027**

|  |  |  |
| --- | --- | --- |
| Energy per atom in eV | Fe | Cr |
| Primitive | -8.25654064 | -9.50756513 |
| Unit Cell | -8.2571397 | -9.52157098 |
| Difference between Primitive and Unit cell | -0.01400585 > 1meV | -0.00059906 < 1meV |

Since the difference between the energy in Ferromagnetic Iron is less than 1 meV. Primitive cell can be uses for modelling in case of Iron.

In case of Chromium , since it is more than 1 meV, we must use BCC unit cell for modelling in this case.