

```
calculator = Vasp( ismear = 0,  
    sigma      = 0.15,  
    xc         = 'PBE',  
    isif       = 2,  
    encut      = 400,  
    idipol     = 4,  
    dipol      = [0.500, 0.500, 0.500],  
    ialgo      = 38,  
    enaugh     = 650,  
    voskown    = 1,  
    ediff      = 10E-7,  
    lreal      = False,  
    lcharg     = True,  
    lwave      = True,  
    ispin      = 2,  
    kpts       = (5,5,1))
```