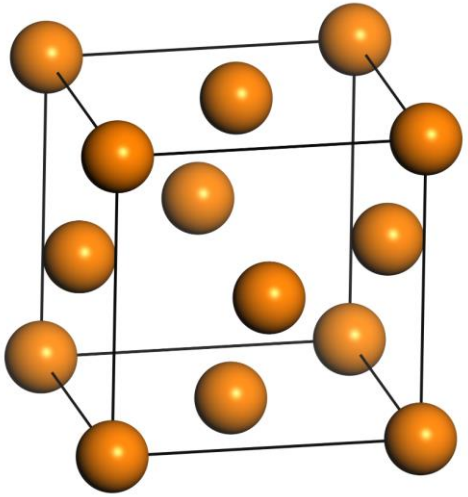
9月25日上机实习安排

1. 高对称FCC Fe_{13}团簇的建模
2. 单层石墨烯@Ni(111)表面的建模
3. 用GaussView结合Materials Studio软件进行$Ni_3(HITP)_2$二维单层膜的建模

徐旌凯同学针对如何构建$Ni_3(HITP)_2$分子片段进行PPT展示！

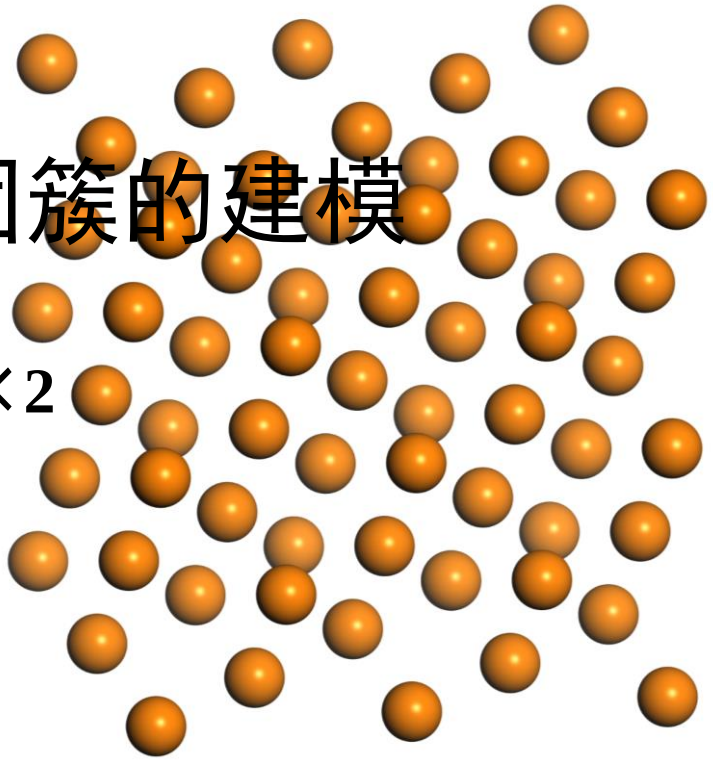
余下时间上机操作（同学们、老师一起讨论操作），下课前10 min告之完成情况

1. 高对称FCC Fe_{13}团簇的建模



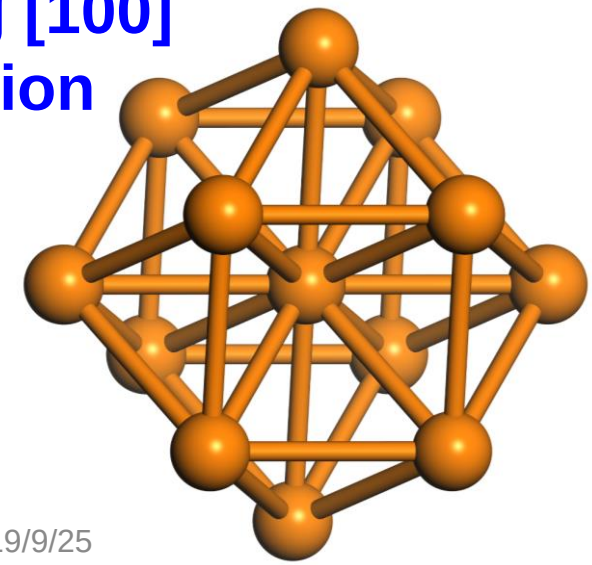
1. FCC Fe supercell 2×2

2. Nonperiodic structure

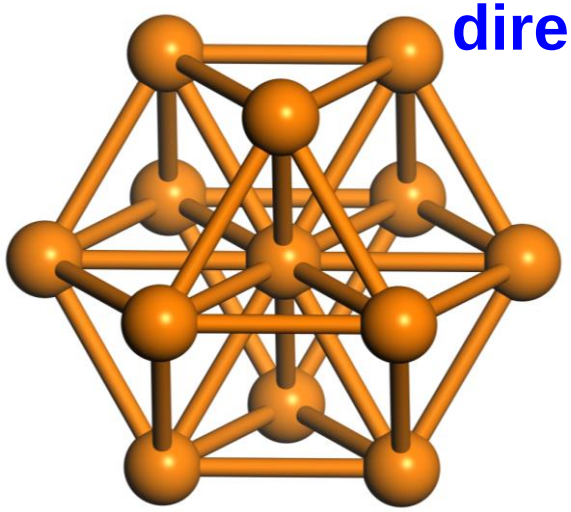


Cut atoms

Along [100] direction

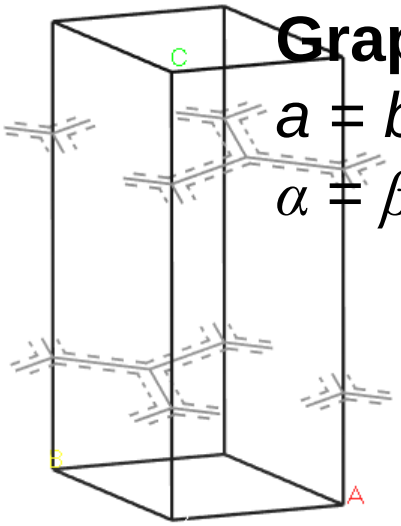


Along [111] direction



2. Graphene@Ni(111)表面的建模

Import crystal structures



Graphite

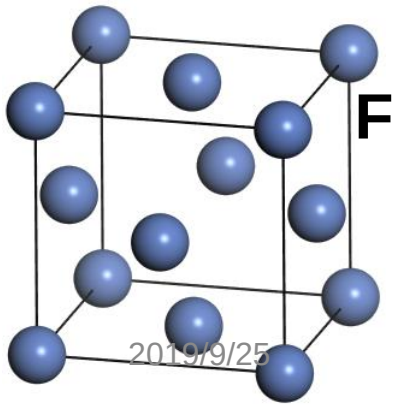
$a = b = 2.460$ Å, $c = 6.8$ Å

$\alpha = \beta = 90^\circ$, $\gamma = 120^\circ$

Ni(111) surface

$a = b = 4.984$ Å

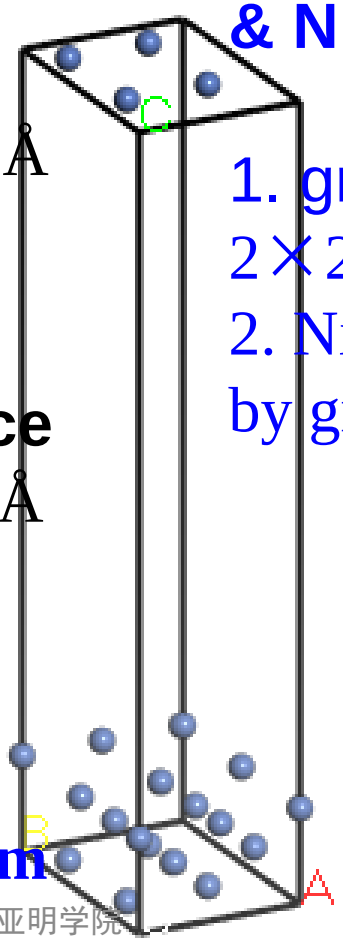
$\gamma = 120^\circ$



FCC Ni

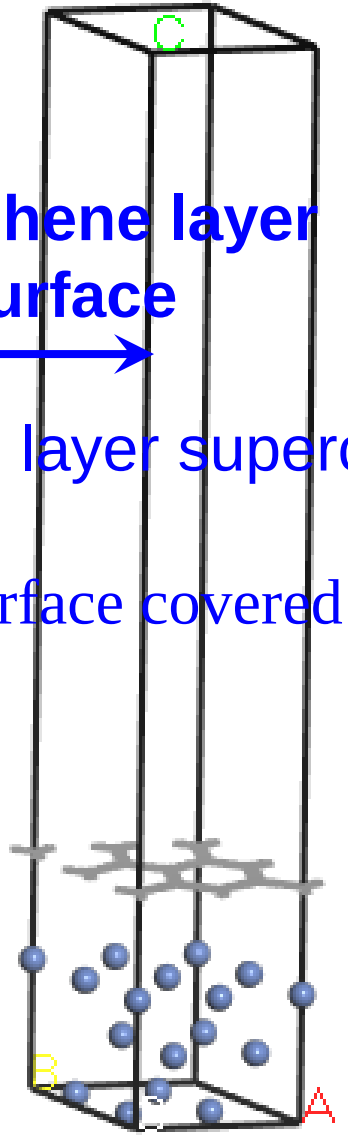
1. Cut Ni(111)

2. Add 30 Å-vacuum layer (re-orient)



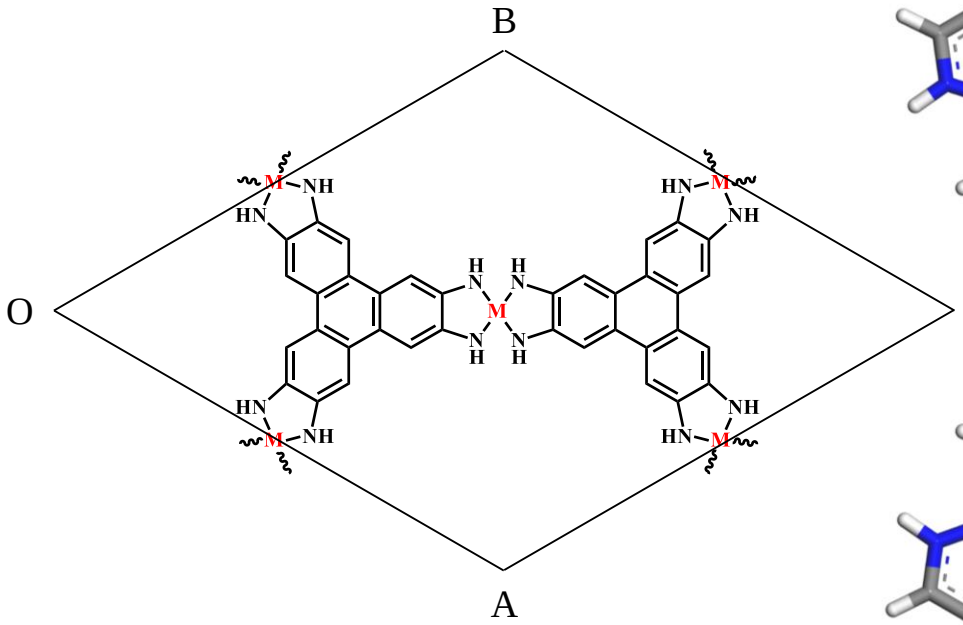
Match graphene layer & Ni(111) surface

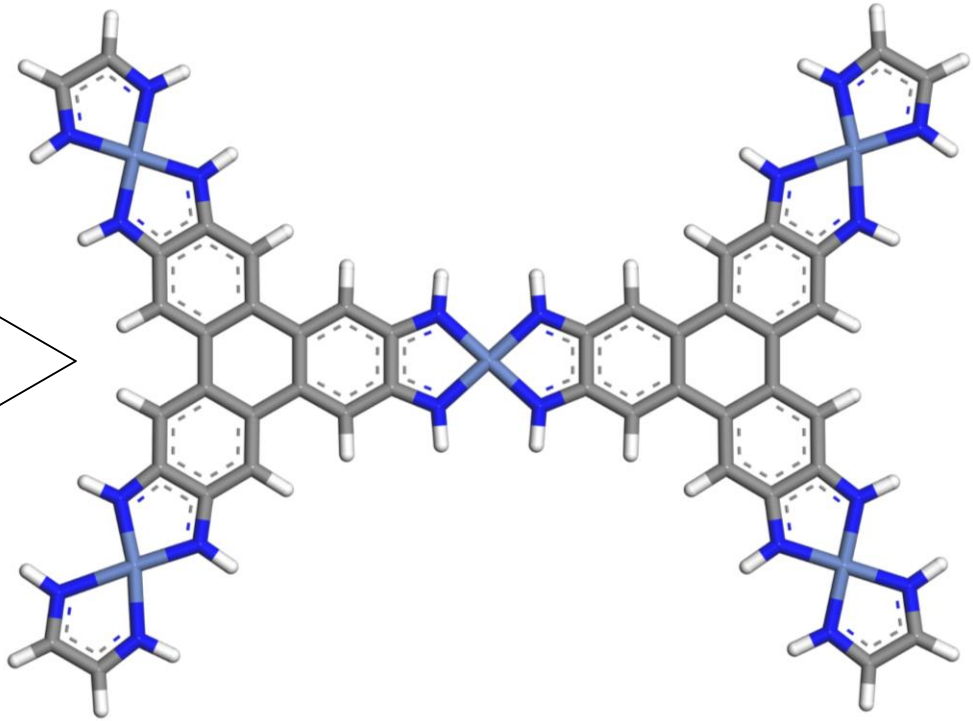
1. graphene layer superce
2×2
2. Ni(111) surface covered by graphene



3. $Ni_3(HITP)_2$二维单层膜的建模

- Draw $Ni_3(HITP)_2$ formula unit by using GaussView





3. $Ni_3(HITP)_2$二维单层膜的建模

- Build crystal by using Materials Studio