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MDI505Homework3

In [1]:
```
import numpy as np
import matplotlib.pyplot as plt
%matplotlib inline
```

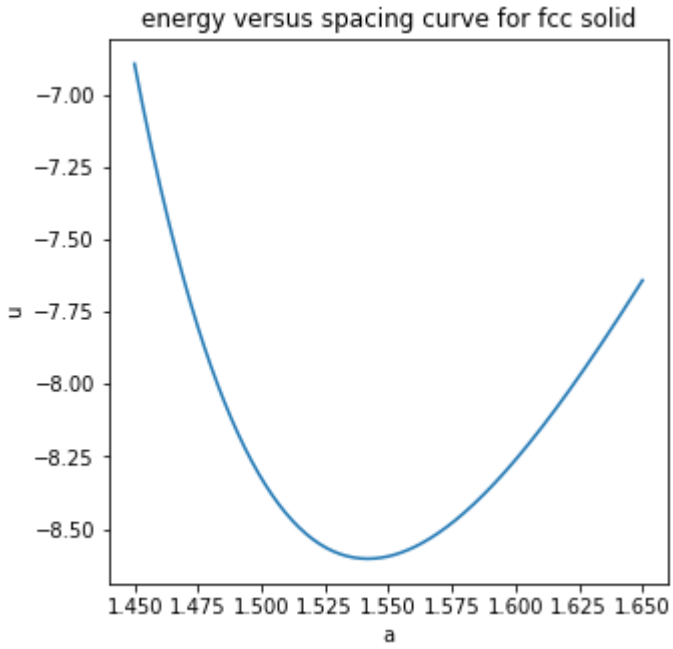
In [2]:
```
def energy(a, nc, crystal_type='bcc'):
    if crystal_type == 'fcc':
        n = 4
        r = np.array([[0, 0, 0], [0, 0.5, 0.5], [0.5, 0, 0.5], [0.5, 0.5, 0]])
    elif crystal_type == 'bcc':
        n = 2
        r = np.array([[0, 0, 0], [0.5, 0.5, 0.5]])

    ucell = 0

    for k in range(-nc, nc):
        for l in range(-nc, nc):
            for m in range(-nc, nc):
                for i in range(n):
                    for j in range(n):
                        dist = a * np.sqrt((k+r[j, 0]-r[i, 0])**2 + (l+r[j, 1]
-r[i, 1])**2 + (m+r[j, 2]-r[i, 2])**2)
                        if dist > 0:
                            u = 2 * (1/dist**12 - 1/dist**6)
                        else:
                            u = 0
                        ucell += u

    ucell /= n

    return ucell
```

In [3]:
```
def plot(a, u, crystal_type):
    plt.figure(figsize=(5, 5))
    plt.plot(a, u)
    plt.xlabel('a')
    plt.ylabel('u')
    plt.title('energy versus spacing curve for ' + crystal_type + ' solid')
    plt.show()
```

Plot the energy versus spacing curve for FCC solid

In [4]:
```
a = np.linspace(1.45, 1.65, 300)
ucell = []
for space in a:
    ucell.append(energy(space, 6, 'fcc'))
```

In [5]:
```
plot(a, ucell, 'fcc')
```



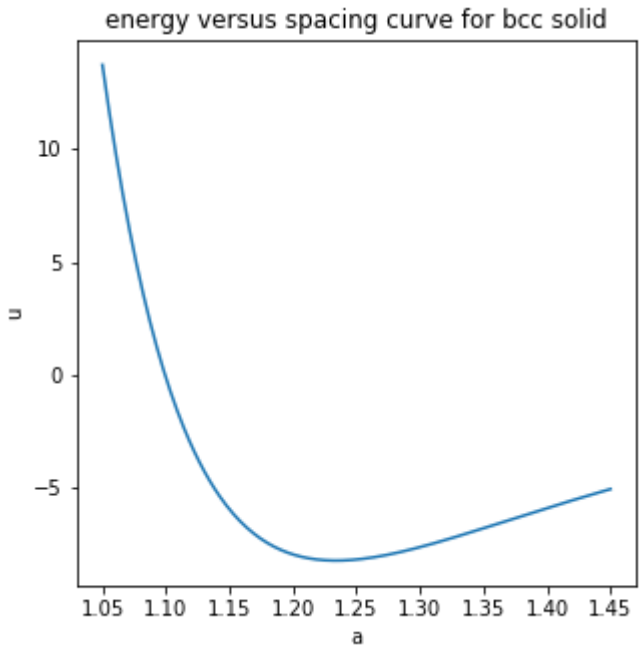
In [6]:
```
u0 = min(ucell)
a0 = a[ucell.index(u0)]
print('For fcc solid')
print('a0=', round(a0, 3))
print('u0=', round(u0, 3))
```

```
For fcc solid
a0= 1.542
u0= -8.603
```

Plot the energy versus spacing curve for BCC solid

In [7]:
```
a = np.linspace(1.05, 1.45, 300)
ucell = []
for space in a:
    ucell.append(energy(space, 6, 'bcc'))
```

In [8]:
```
plot(a, ucell, 'bcc')
```



In [10]:
```
u0 = min(ucell)
a0 = a[ucell.index(u0)]
print('For bcc solid')
print('a0=', round(a0, 3))
print('u0=', round(u0))
```

```
For bcc solid
a0= 1.233
u0= -8.0
```

Compare energetics for both fcc and bcc at the equilibrium as a function of the cutoff distance.

For the FCC solid, the equilibruim is $a_0 \approx 1.542\sigma$ and $u_0 \approx -8.603\epsilon$. And for the BCC solid, the equilibrium is $a_0 \approx 1.233\sigma$ and $u_0 \approx -8.0\epsilon$. Therefore, the a_0 and u_0 for BCC is smaller at the equilibruim.

In [ ]: