In [55]:
```
#Task 1
```

In [56]:
```
import pandas as pd
import numpy as np
```

In [57]:
```
data = pd.read_csv('/Users/gaotianyi/Desktop/coding test/eos.csv')
V = data['Volume (A^3/atom)'].values
E = data['Energy (eV/atom)'].values
```

In [58]:
```
V = np.array([17.9358497960000, 18.4963051840000, 19.0683159480000, 19.65
E = np.array([-2.59094217375, -2.603891814375, -2.610287264375, -2.610762
```

In [59]:
```
def energy_volume_equation(V, a, b, c, d):
    return a + b * V**(-2/3) + c * V**(-4/3) + d * V**(-2)
```

In [60]:
```
from scipy.optimize import curve_fit
```

In [61]:
```
params, _ = curve_fit(energy_volume_equation, V, E, p0 = [E.min(), 1, 1,
#fitting parameters
a, b, c, d = params
print(f"a = {a:.13f}")
print(f"b = {b:.13f}")
print(f"c = {c:.13f}")
print(f"d = {d:.13f}")
```

```
a = 2.5127759357659
b = -61.3468543311741
c = 84.3580903235784
d = 660.3355995361577
```

In [62]:
```
params, _ = curve_fit(energy_volume_equation, V, E, p0 = [E.min(), 5, 5,
#fitting parameters
a, b, c, d = params
print(f"a = {a:.13f}")
print(f"b = {b:.13f}")
print(f"c = {c:.13f}")
print(f"d = {d:.13f}")
```

```
a = 2.5127734027969
b = -61.3467990974659
c = 84.3576892245220
d = 660.3365695401521
```

In [63]:
```
params, _ = curve_fit(energy_volume_equation, V, E, p0 = [E.min(), 10, 10
```

In [64]:
```
#fitting parameters
a, b, c, d = params
print(f"a = {a:.13f}")
print(f"b = {b:.13f}")
print(f"c = {c:.13f}")
print(f"d = {d:.13f}")
```

```
a = 2.5127739867257
b = -61.3468117909906
c = 84.3577811153304
d = 660.3363480096118
```

In [65]:
```
#range
print(f":{V.min():.3f} - {V.max():.3f}A^3/atom")
```

```
:17.936 - 21.474A^3/atom
```

In [66]:
```
E_fitted = energy_volume_equation(V, a, b, c, d)
```

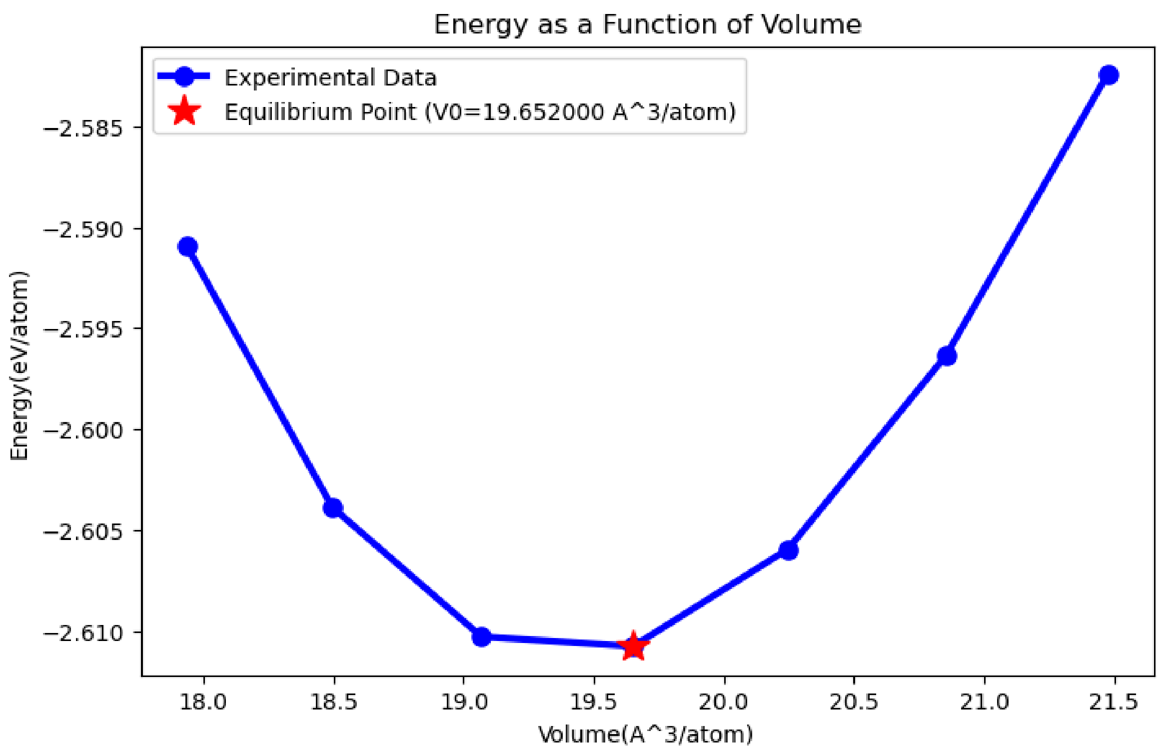
In [67]:
```
min_index = np.argmin(E_fitted)
V0 = V[min_index]
E0_min = E_fitted[min_index]
print(f"Equilibrium volume = {V0:.6f} A^3/atom")
```

```
Equilibrium volume = 19.652000 A^3/atom
```

In [68]:
```
#Task 2
```

In [69]:
```
import matplotlib.pyplot as plt
```

In [70]:
```
plt.figure(figsize=(8, 5))
plt.plot(V, E, 'bo-', markersize=8, linewidth=3, label='Experimental Data
E_fitted = energy_volume_equation(V, a, b, c, d)
V0 = V[np.argmin(E_fitted)]
E0 = np.min(E_fitted)
plt.plot(V0, E0, 'r*', markersize=15, label=f'Equilibrium Point (V0={V0:.
plt.xlabel('Volume(A^3/atom)')
plt.ylabel('Energy(eV/atom)')
plt.title('Energy as a Function of Volume')
plt.legend();
```



In [ ]: