MS4023 : Electronic Structures and Atomistic Modeling

LAB EXERCISE - II

CO23BTECH11021

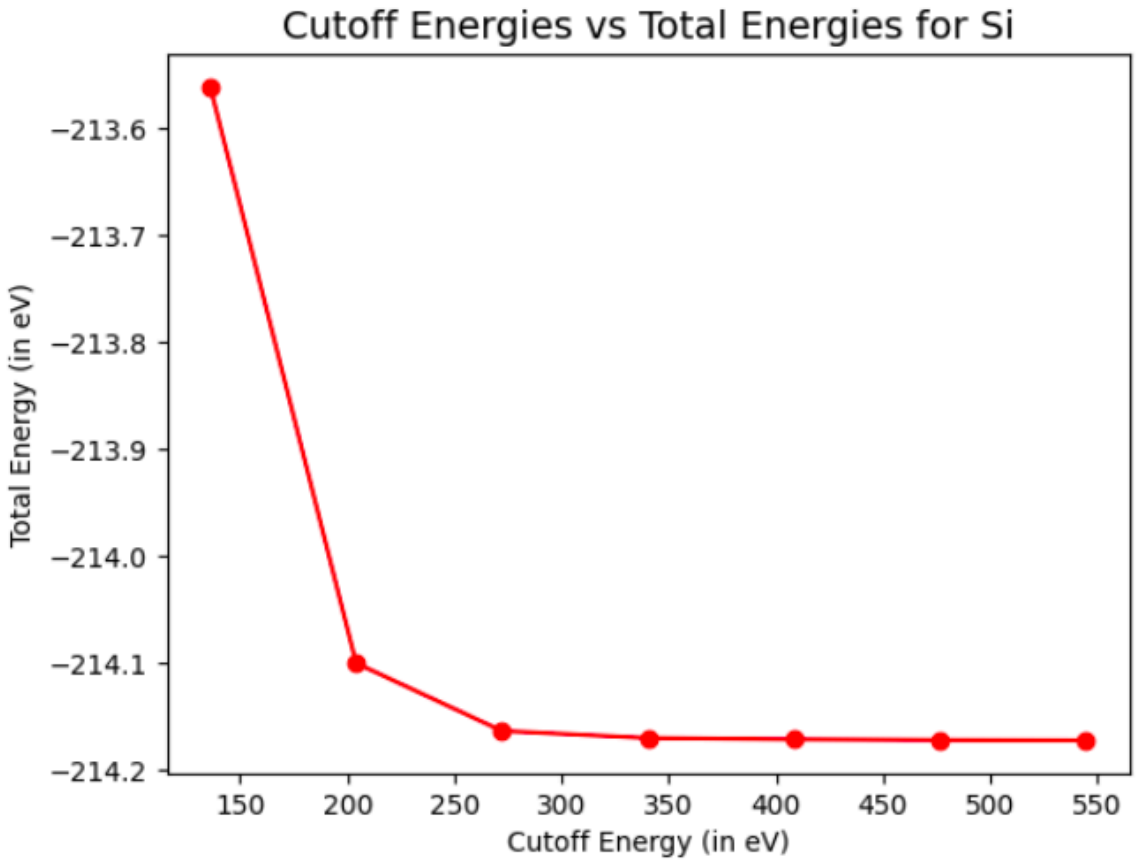
Si

pwd : /home/co23btech11021/testDIrectory/Jan2025/exercise2_Si/

1. Table

Cutoff Energy (in eV)	**Total Energy** (in eV)	**No. of K points**	**No. of G vectors**	**SCF Iterations**
136.057	-213.5616	28	1139	5
204.0856	-214.1002	28	2085	5
272.1141	-214.1636	28	3287	5
340.1426	-214.1702	28	4573	5
408.1711	-214.1714	28	5961	5
476.1996	-214.1721	28	7631	5
544.2282	-214.1724	28	9257	5

2. Plot



3. E_cutoff vs Convergence

The total energy for Si converges (difference between the present energy and previous energy is less than 0.01 eV) at the value of the **cutoff energy = 340.1426 eV** or **25 Ry**.

4. Total energy vs E_cutoff

The total energy **decreases monotonically** with the increase in the cutoff energies.

5. Runtime vs E_cutoff

Cutoff Energy (in eV)	**Runtime(WALL)** (in s)
136.057	0.30
204.0856	0.56
272.1141	0.94
340.1426	1
408.1711	1.26
476.1996	2.01
544.2282	2.13

With the increase in the value of cutoff energy, the **WALL runtime** also **increased**.

6. Variation of K points, G vectors

Irrespective of the cutoff energy, the number of **K points always remains the same**. The number of **G vectors increases** with the value of the cutoff energy. Number of **SCF iterations** also were **constant**.

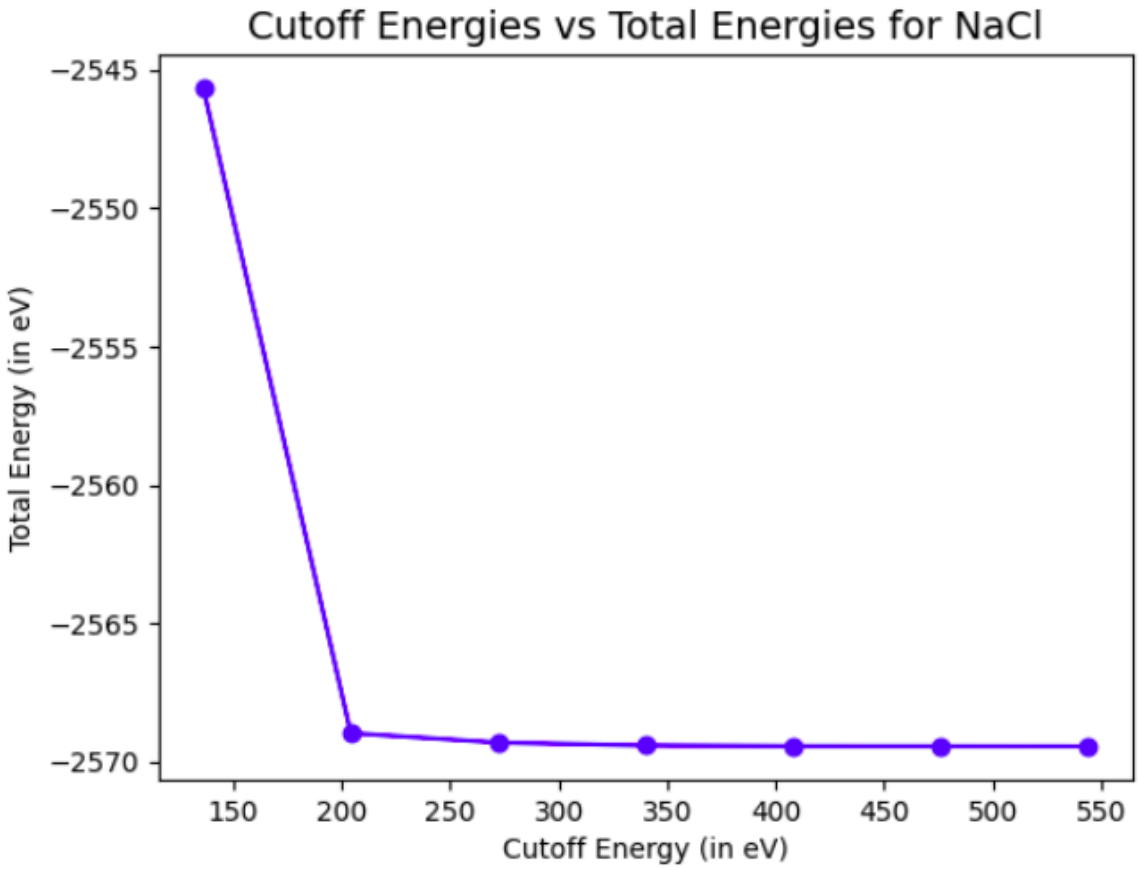
NaCl

pwd : /home/co23btech11021/testDIrectory/Jan2025/exercise2_NaCl/

1. Table

Cutoff Energy (in eV)	**Total Energy** (in eV)	**No. of K points**	**No. of G vectors**	**SCF Iterations**
136.057	-2545.6515	28	1243	6
204.0856	-2568.9731	28	2397	7
272.1141	-2569.3138	28	3695	6
340.1426	-2569.4175	28	5029	7
408.1711	-2569.4437	28	6615	7
476.1996	-2569.4461	28	8363	7
544.2282	-2569.4498	28	10177	7

2. Plot



3. E_cutoff vs Convergence

The total energy for NaCl **converges** (difference between the present energy and previous energy is less than 0.01 eV) at the value of the **cutoff energy = 476.1996 eV** or **35 Ry**.

4. Total energy vs E_cutoff

The total energy **decreases monotonically** with the increase in the cutoff energies.

5. Runtime vs E_cutoff

Cutoff Energy (in eV)	**Runtime(WALL)** (in s)
136.057	0.93
204.0856	2.38
272.1141	3.57
340.1426	4.35
408.1711	5.14
476.1996	6.62
544.2282	5.69

With the increase in the value of cutoff energy, the WALL **runtime also increased.** However, a **small exception** was observed at **E_cutoff = 40 Ry**

6. Variation of K points and G vectors

Number of **K points** were the **same** but the number of **G vectors increased** with the values of E_cutoff. The number of **SCF iterations** were **7** for most of the cases.