

Task-4: Band Structure of Graphene Nanoribbon

Armchair Graphene Nanoribbon- AGNR

Matlab Code:

```
clc; close all; clear all;
```

```
%% Parameters
```

```
t0 = 2.7;
```

```
a = 0.142e-9;
```

```
AGNR=5;
```

```
n = 2*AGNR;
```

```
N=1000;
```

```
k = linspace(-pi/a,pi/a,N);
```

```
%% Hamiltonian Form
```

```
Hnn = zeros(n,n);
```

```
Hnn(1,2)=-t0;
```

```
Hnn(1,n) = -t0;
```

```
Hnn(n,1) = -t0;
```

```
Hnn(n,n-1) = -t0;
```

```
for i = 2:n-1
```

```
    Hnn(i,i-1) = -t0;
```

```
    Hnn(i,i+1) = -t0;
```

```
    if (i<(n/2) && (rem(i,2))~=0)
```

```
        Hnn(i,n-i+1) = -t0;
```

```
        Hnn(n-i+1,i) = -t0;
```

```
    end
```

```
end
```

```
HnnR = zeros(n,n);
```

```
HnnL = zeros(n,n);
```

```
for i = 1:n
```

```
    if(i<=(n/2) && (rem(i,2))==0)
```

```
        HnnR(n-i+1,i) = -t0;
```

```
    end
```

```
end
```

```
HnnL = HnnR';
```

```
%% Eneergy Findings
```

```
E = zeros(n,length(k));
```

```
for p = 1:length(k)
```

```
    H_final = Hnn + HnnR.*exp((1i).*k(p)*a) + HnnL.*exp(-(1i).*k(p)*a);
```

```
    V = eig(H_final);
```

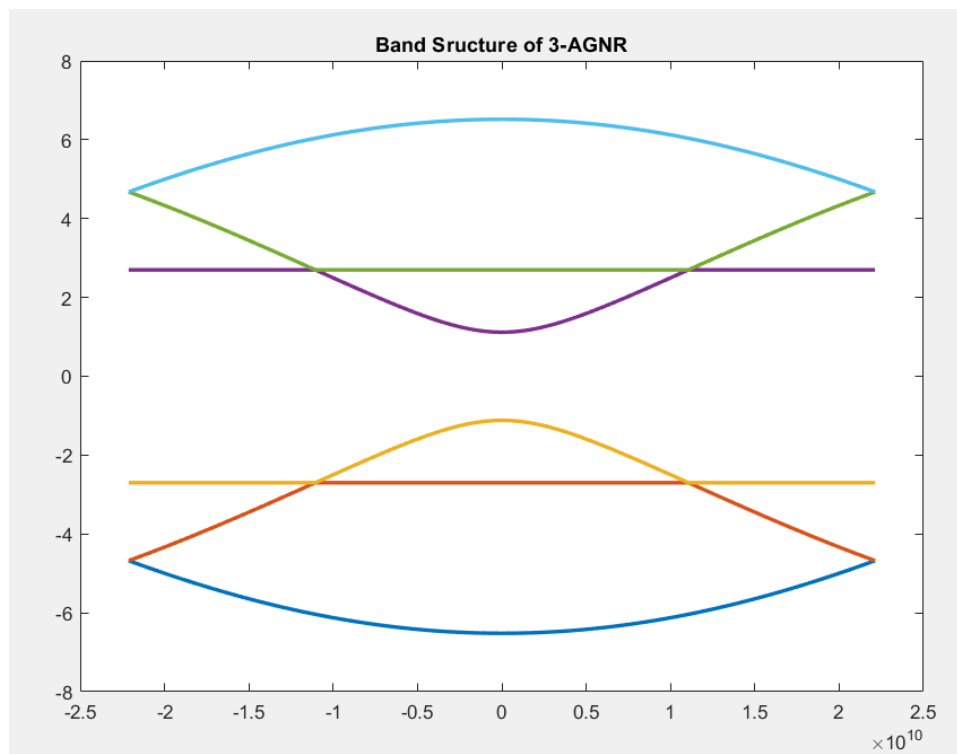
```

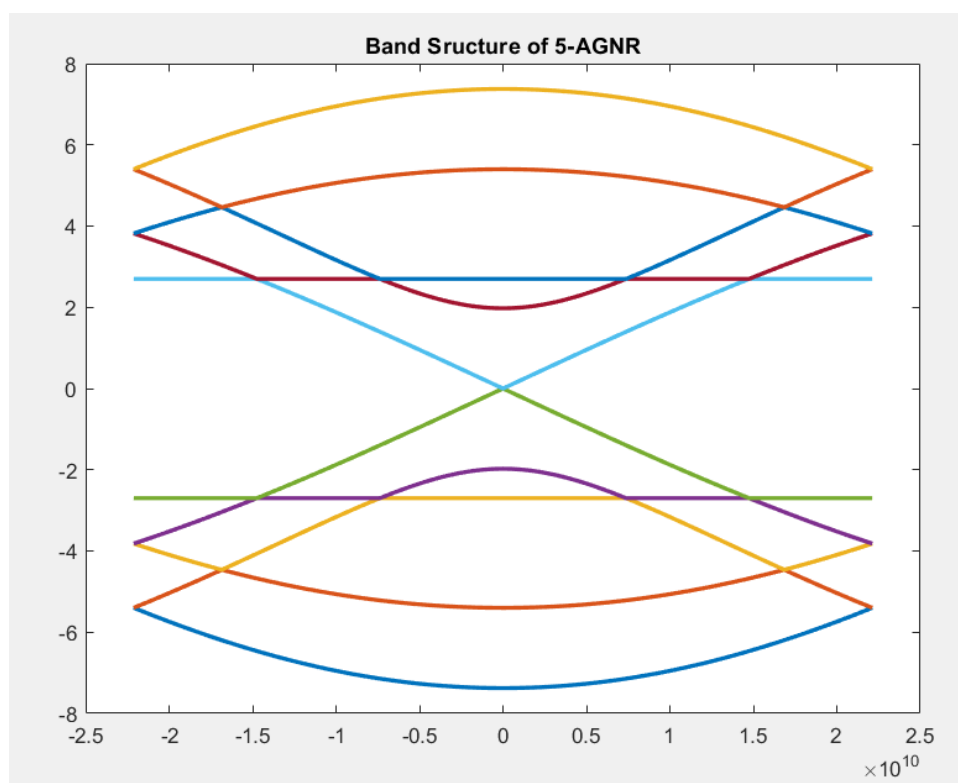
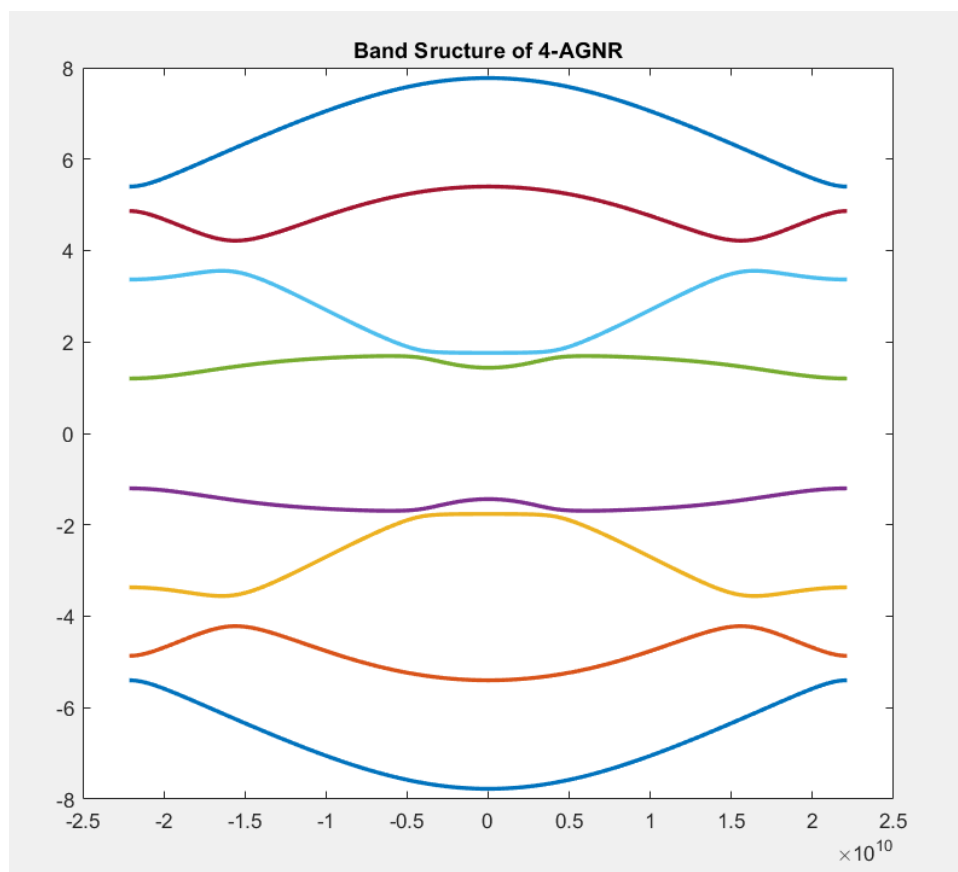
    E(:,p) = V;
end

%% Ploting
for i = 1:n
    plot(k,E(i,:), 'Linewidth',2);
    hold on
    title(" Band Structure of " + AGNR + "-AGNR ")
end

```

Plot:





Zigzag Graphene Nanoribbon- ZGNR

Matlab Code:

```
clc; close all; clear all;
```

```
%% Parameters
```

```
t0 = 2.7;
```

```
a0 = 0.142e-9;
```

```
b = sqrt(3)*a0;
```

```
N=1000;
```

```
k = linspace(-pi/b,pi/b,N);
```

```
ZGNR=8;
```

```
n=ZGNR;
```

```
%% Hamiltonian Form
```

```
Hnn = zeros(n,n);
```

```
Hnn(1,2) = -t0;
```

```
Hnn(n,n-1) = -t0;
```

```
for i = 2:n-1
```

```
    Hnn(i,i-1) = -t0;
```

```
    Hnn(i,i+1) = -t0;
```

```
end
```

```
HnnR = zeros(n,n);
```

```
HnnR(1,2) = -t0;
```

```
HnnR(n,n-1) = -t0;
```

```
for i = 4:4:n-1
```

```
    HnnR(i,i-1) = -t0;
```

```
    HnnR(i+1,i+2) = -t0;
```

```
end
```

```
HnnL = HnnR';
```

```
%% Energy Finding
```

```
E = zeros(n,length(k));
```

```
for p = 1:length(k)
```

```
    H_final = Hnn + HnnR.*exp((1i).*k(p)*b) + HnnL.*exp(-(1i).*k(p)*b);
```

```
    V = eig(H_final);
```

```
    E(:,p) = V;
```

```
end
```

```
%% Plotting
```

```
for i = 1:n
```

```
    plot(k,E(i,:), 'Linewidth',2);
```

```
    hold on
```

```
    title(" Band Sructure of " + ZGNR + " - ZGNR ")
```

```
End
```

Plot:

