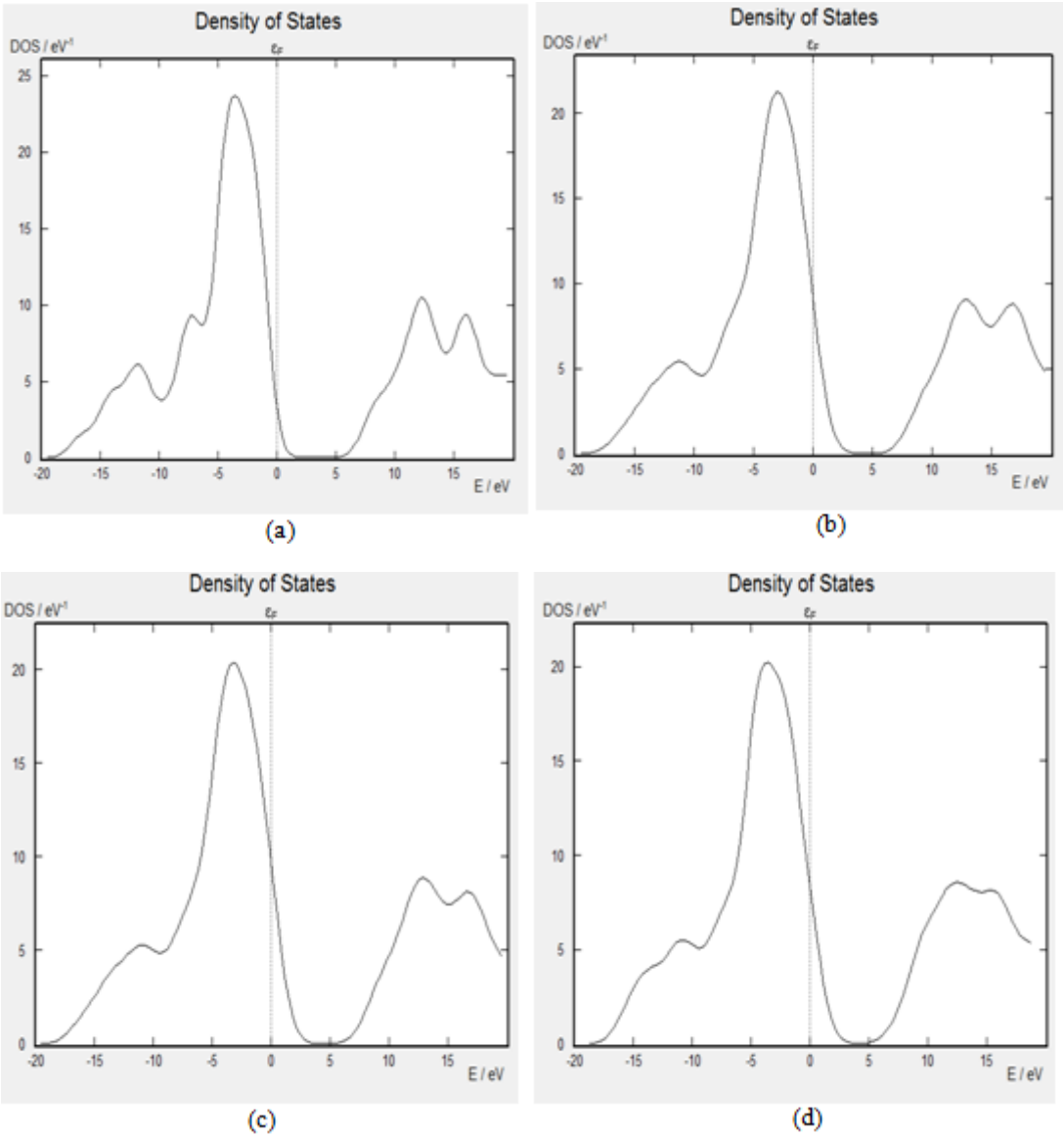
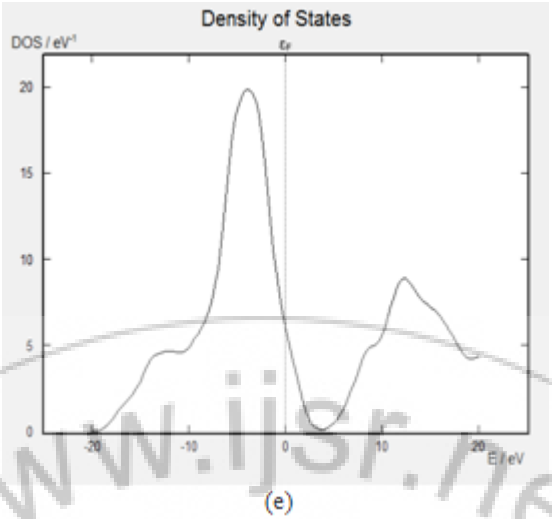
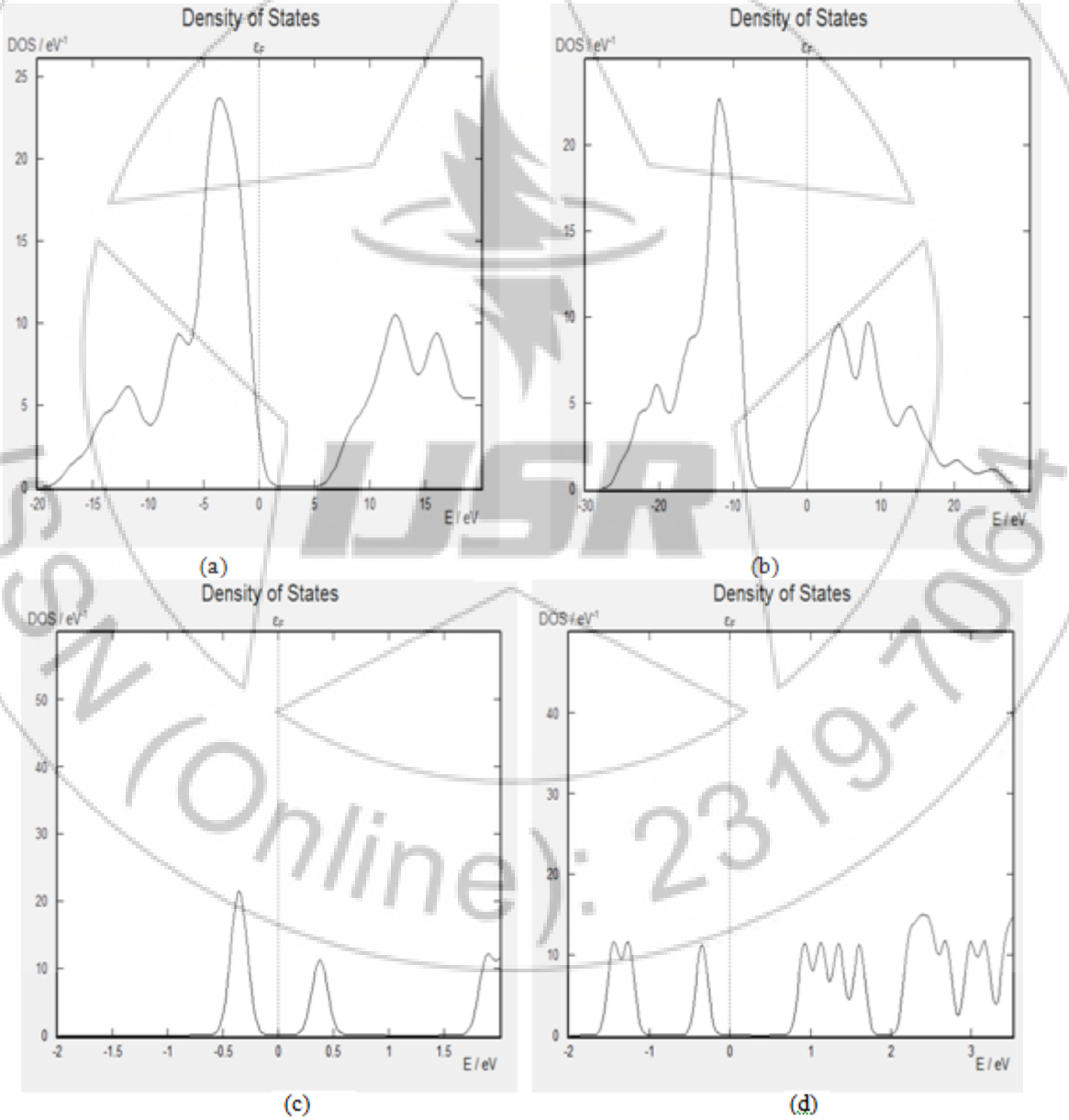
with the increase in number of Al and P atoms .Now , this bulk Sillicon nanowire is doped with three Al atom , the graph shows a high peak which is at 20.2 DOS/ev in y axis and -2.8 E/ev on x axis . There are two peaks on the right side which appears on 5.5, 4 DOS/ev on y axis resp. and -11,14 E/ev in x axis resp. But there are two peaks on the left side is present on 8.7, 8 DOS/ev on axis y and -11, 15.4 E/ev in x axis resp. And then this bulk Sillicon nanowire is doped with four Al atom , the graph shows a high peak which is at 19.4 DOS/ev in y axis and -4.7 E/ev on x axis . There are two peaks on the right side which appears on 3.7, 5.4 DOS/ev on y axis resp. and -13,-15 E/ev in x axis resp. But there are two peaks on the left side is present on 7.4, 8.2 DOS/ev on y axis and 10 , 11.7 E/ev in x axis resp. . The left side of Fermi level is denser which clearly indicates high metallic nature. Now it's the turn for phosphorous doping on Sillicon nanowire . When this bulk Sillicon nanowire is doped with a P atom, the graph shows a high peak which is at 22.67 DOS/ev in y axis and -11 E/ev on x axis. There are three peaks on the right side appears on 4.4 , 6 , 8.7 DOS/ev on y axis and -11,-17,-20.7 E/ev in x axis resp. But there are 5 peaks on the left side is present on 9.5,9.7,4.7,1.6,1.08 DOS/ev on y axis and 4,9.6,17,20, 25 E/ev in x axis resp. Now this bulk Sillicon nanowire is doped with two P atoms, the graph becomes very dense and it clearly defends very high metallic nature. There are three peaks on both sides of femi level . The peaks appears on 23, 6.2, 9.2 DOS/ev on one side of Fermi level which is at -0.3, -12.5, -21.6 in x axis .But when this Sillicon nanowire is doped with three P atoms, we observe one side of Fermi level has three peaks, the graph shows peaks which is at -1.3,-0.5,-1.7 DOS/ev in y axis and 10.3,10.4,10.2E/ev on x axis resp . But on the other side, there are many small peaks. We observe lot of distorted peaks on the valence band which defends it is metallic .Finally this bulk Sillicon nanowire is doped with four P atoms , the graph shows a three peaks on one side of fermi level which is at 7.5, 12.6,19.8 DOS/ev in y axis and other side has around seven peaks which appears on 9.6 , 10.4 , 4.7 ,5.4,4.8,1.8,1 DOS/ev .Here , we see small peaks raising up .As usual there is presence of more peaks but now the peaks are getting distorted on both sides because of increase in number of electrons of Aluminium and phosphrous atoms .

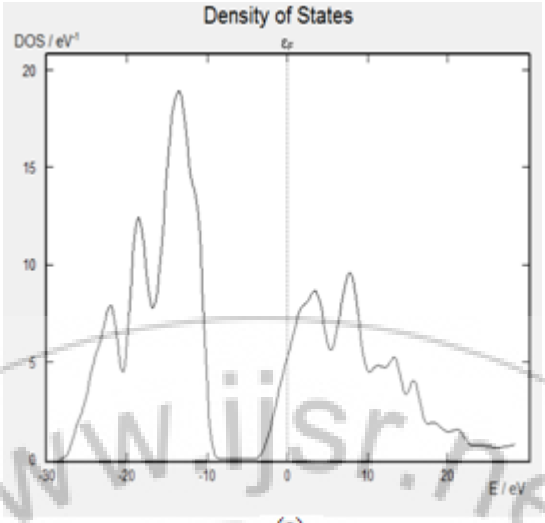




(e)

Figure 6: The Density of States of Si nanowires (a) SiNW without doping , (b) SiNW doped with 1 Al atom , (c) SiNW doped with 2 Al atoms , (d) SiNW doped with 3 Al atoms and (e) SiNW Doped with 4 Al atoms





(e)

Figure 7: The Density of structures of Si nanowires (a) SiNW without doping , (b) SiNW doped with 1 P atom , (c) SiNW doped with 2 P atoms , (d) SiNW doped with 3 P atoms and (e) SiNW Doped with 4 P atoms

4. Conclusions

After analysing the structural and electronics properties of Sillicon nanowire, we can conclude that in case of structural property, if total energy is maximum then the structure is least stable. So we can say that total energy is inversely proportional to stability with the increase of doping Al and P atoms, total energy is increasing. In density of states, we clearly see the decline in DOS/Ev with the increase of doping Al and P atoms. But the graph was getting denser and crowded with conduction lines as the metallic property is increasing. Finally , in Bandstructure , we observe that band gap gets hidden because of crowded conduction lines while doping it with Al and P atoms which depicts the increase of metallic nature as earlier in case of Si NW , there was small band gap available depicting semiconductor property.

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