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## Effect of N and B-doping on the electronic properties of 6,6,12-graphyne

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In this study we investigate the electronic properties of intrinsic and N and B-doping graphyne 6,6,12 using SIESTA code based on density functional theory. The results show that the intrinsic graphyne 6,6,12 is a semi –metal with Dirac cones between r to X' and at X symmetry point. Doping N to the graphyne 6,6,12 changes it from semi-metal to a n-type semiconductor with indirect band gap. Doping B to the graphyne 6,6,12 changes it from semi-metal to metal. These results can be used in making high- performance nano-electronic components based on graphyne.

### Biography

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