Rational edge functionalization of zigzag graphene nanoribbons for band gap opening and induced aromaticity patterns.

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Tuning the band gap of graphene nanoribbons by chemical edge functionalization is a promising approach towards future electronic devices based on graphene.[1] The band gap is closely related to the aromaticity distribution[2] and therefore tailoring the aromaticity patterns is a rational way for controlling the band gap. In the present work, a way to open a band gap on zigzag graphene nanoribbons by selective edge functionalization is shown. Based on Clar's Sextet Theory,[3] additional hydrogen at the edges, oxygen and tailored edges are suggested as possible ways for inducing aromaticity patterns and therefore opening the band gap. It demonstrates that rational tuning of the band gap can be performed, allowing the application of graphene nanoribbons in semiconducting devices. The electronic structure and the aromaticity distribution are studied using DFT calculations and through a series of delocalisation and geometry analysis methods, like the six-centre index (SCI) and the mean bond length (MBL) geometry descriptor.[4]

References

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