A theoretical study of graphene nanoribbons

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Zig-zag nanoribbon
Armchair nanoribbon (odd)
Armchair nanoribbon (even)
Chevron type nanoribbon
Single site functionalisation
Two site functionalisation
- Investigate the effect of functional group density
- Determine the impact on mechanical properties
- Review different computational methods for these purposes
Thank you for listening

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