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Effects of Position and Shape of Atomic Defects on the Band Gap of Graphene Nano-Ribbon Superlattices

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Abstract : In this work, we study the behavior of introducing atomic size vacancy in a graphene nanoribbon superlattice. Our investigations are based on the density functional theory (DFT) with the Local Density Approximation in Atomistix Toolkit (ATK). We show that, in addition to its shape, the position of vacancy has a major impact on the electrical properties of a graphene nanoribbon superlattice. We show that the band gap of an armchair graphene nanoribbon may be tuned by introducing an appropriate periodic pattern of vacancies. The band gap changes in a zig-zag manner similar to the variation of the band gap of a graphene nanoribbon by changing its width.

Keywords : AGNR, antidot, atomistic toolKit, vacancy
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