Theoretical investigations on the transport properties of graphene nanoribbons

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Recent advancements in the production techniques of novel materials based on graphene[1] allow us to envision next-generation electronic devices with active components based on nanostructured carbon. In particular, materials based on graphene nanoribbons (GNRs) are expected to play a crucial role in this sense due to the dimensional confinement which allows a fine-tuning of the electronic and, consequently, transport properties [2]. Although transport properties of GNRs have already been investigated in detail [3], a comprehensive understanding of the relationships between morphological features and quantum transport is still missing. Especially, this issue concerns the role of defects, edge terminations and structural details beyond high-symmetric morphologies. In this work we analyze and characterize, by means of density functional theory and non-equilibrium Green function calculations, the electronic and transport properties of defect-free, defected and functionalized graphene nanoribbons. Our methodology integrates valence bond (VB) concepts and Clar sextet theory [4,5] into electronic structure calculations by evaluating properties such as stability, band structure and molecular orbitals of the systems under investigation.

References

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[4] Baldoni, M; Sgamellotti, A; Mercuri, F, Org. Lett., **9** (2007) 4267.
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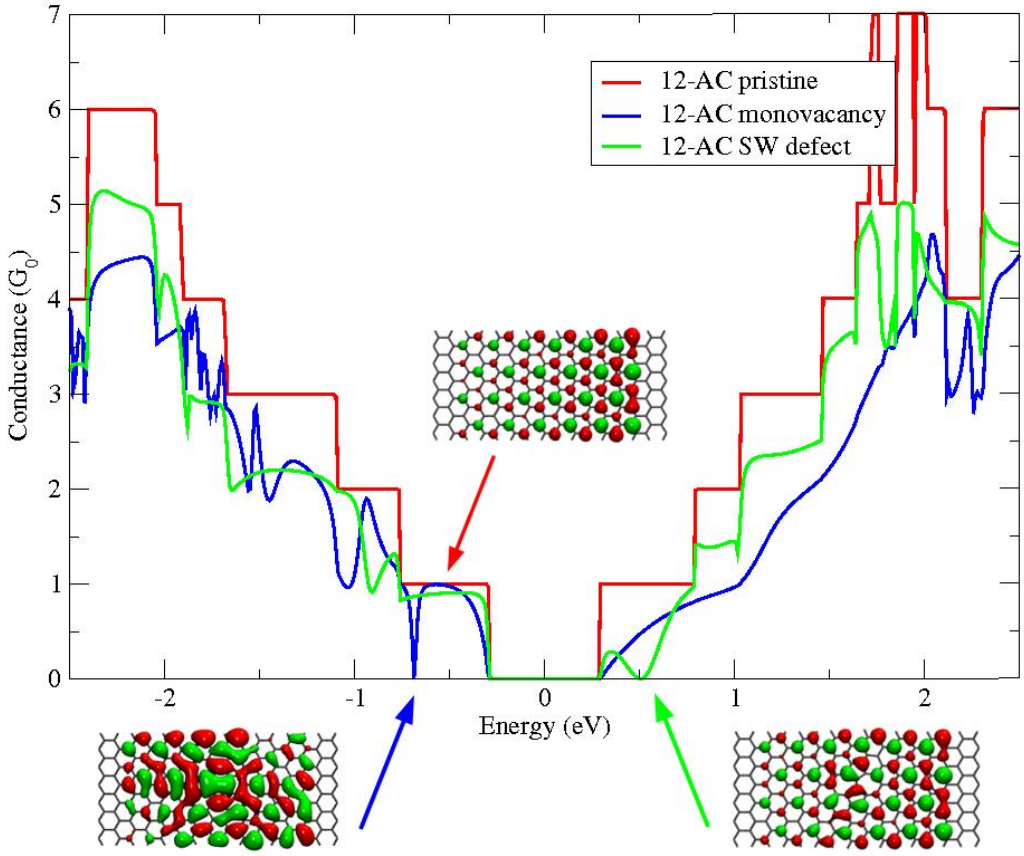
Figures



Transmission spectra of armchair-edge 12-AC pristine (red lines), with monovacancy defect (blue lines) and with Stone-Wales defect (green lines). Transmission eigenstates are also depicted above the correspondin transmission plateau.