

Ab initio Real-Space Study of Free-Standing and Au-Supported Graphene Dots and Nanoribbons

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Abstract

We have examined recently in a series of papers¹⁻⁴ the electronic, aromatic and transport properties of graphene and graphene based structures, as well as the interrelation of these properties, using simple, transparent and very efficient real space models and suitable first principles density functional theory (DFT) methods. Novel results and understanding have been obtained (see Fig. 1) and their interrelation was established¹⁻⁴.

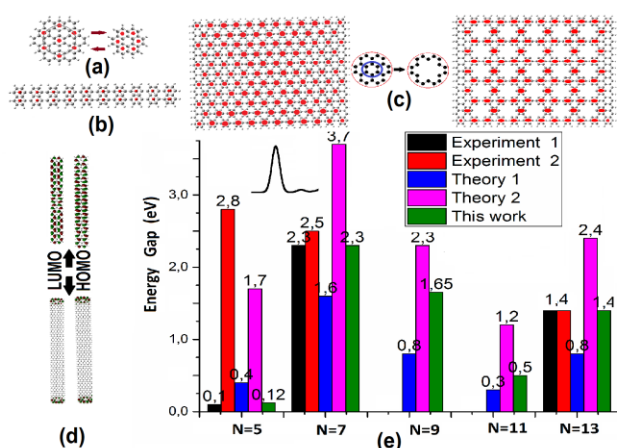


Figure 1: Aromaticity Patterns of graphene and graphene based structures (a), (b), (c)¹⁻³; HOMO LUMO orbitals (d)⁴; and STS gaps (e) for the 5,7,9,11,13 AGNRs⁴.

For atomically precise armchair graphene nanoribbons (AGNRs) we have illustrated⁴ that the existing large discrepancies in the literature for the energy gap, which in some

cases are more than 300%, as shown in Fig.1 (e), can be fully bridged and rationalized by time-dependent density functional theory (TDDFT) and/or by the energy separation of the so-called effective HOMO*, LUMO* orbitals, which in contrast to the actual HOMO and LUMO orbitals, are delocalize over the entire length of the AGNRs. We illustrate that neglect of length (in addition to width) dependence of all interrelated properties is the main source of the discrepancies in the literature⁴ for the energy gap as measured by scanning tunnelling spectroscopy (STS). We illustrate here that that the corrections of the STS gap due to the substrate influence (Fig. 2) because of image charge screening are practically negligible, especially when compared to other sources of error, if the STS gap is properly⁴ determined through TDDFT.

References

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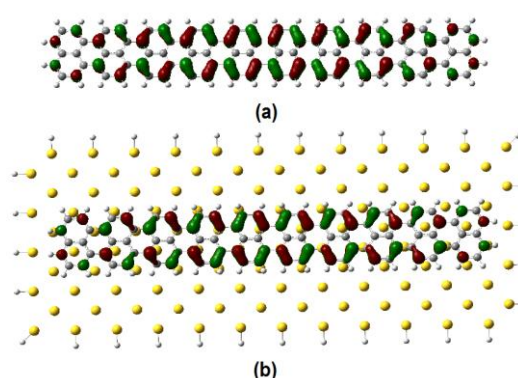


Figure 2: The HOMO orbital of the 5-perylene dimers N=5 AGNR: Free-standing (a) and Au (111) supported (b).