THEORETICAL STUDIES OF NOVEL GRAPHENE BASED NANOSTRUCTURES

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Abstract
Some very appealing methods to open a sizable bandgap in graphene consist in reducing nanoscale dimensions or in forming an ordered array of holes in its honeycomb lattice. Indeed, the reduction of one dimension of graphene leads to graphene nanoribbons (GNRs) [1] while the reduction of the two dimensions leads to graphene quantum dots (GQDs) [2]. As forementioned, a gap can be opened via ordering an array of holes in a graphene lattice as shown in a first theoretical study in 2008. It is called a Graphene Nanomesh (GNM) or a Graphene Anti-dot Lattice (GAL) [3]. First, experimental realizations of GNMs started in 2010 at UCLA [4] and LBNL [5] using a combination of di-block copolymer organization or nanoprinting and selective etching (top-down approach). In this presentation, we will explore the electronic, optics and transport properties of C96 GQDs and its GNM. In Fig. 1a it is possible to obtain C96 GQDs on the gold surface from C96H24(C12H25)6 by physical vapor deposition after heating over 100°C and observed in the experiment. We will show our TB and ab initio calculated results on its electronic structures. Its optical spectra will be performed within an Independant particle picture, with TB as appeared in Fig. 1b. The transport properties will be simulated by ab initio simulated Scanning tunneling microscopy (STM) images (as shown in Fig. (f-g)) as well as tunnel current spectroscopies (STS) and then compared with experimental results (Fig. (c-e)).

References

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[5] Liang, X. G. et al., Nano Lett., 2010, 10, 2454.

Figures

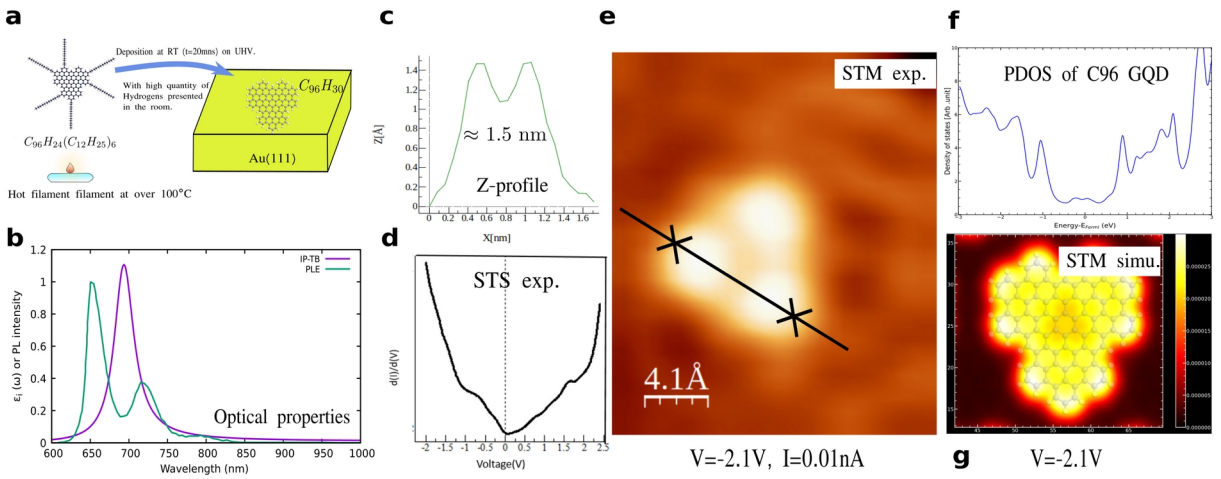

Figure 1: **a**, C96 GQDs's physical vapor deposition conditions and procedures on gold surface. **b**, Photoluminescence spectra of C96C12 and IP-TB spectra of C96's GQD. **c-e**, The height profile, STM and STS experiment results of C96's GQD on Au(111) surface. **f-g**, Projected density of states and STM simulation results of C96's GQD on Au(111) surface.