Photoinduced Processes between Pyrene-Functionalized Silicon Nanocrystals and Carbon Allotropes

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Hybrid nanostructures combining semiconductor quantum dots and carbon allotropes are being developed for applications such as photovoltaics, photo-catalyzed hydrogen production or optoelectronics. Thus, the development of such devices would be pivoted on the fundamental understanding of interactions among the components, with particular regard to the photoinduced processes at the interface.

Silicon nanocrystals (SiNCs) in the quantum size range (2-12 nm) are attracting an increasing interest: on the contrary of bulk silicon, they display a bright emission, which can be tuned from the visible to the near-infrared spectral region by increasing their size [1]. Compared to more traditional quantum dots, such as CdSe, SiNCs offer the following advantages: silicon is abundant, easily available and essentially non toxic, it can form covalent bonds with carbon, thereby offering the possibility of integrating inorganic and organic components in a robust structure. The main drawback is the poor absorption properties of this material, but coupling SiNCs to organic chromophores is a viable route to circumvent this drawback, as recently reported by some of us with a pyrene dye [2].

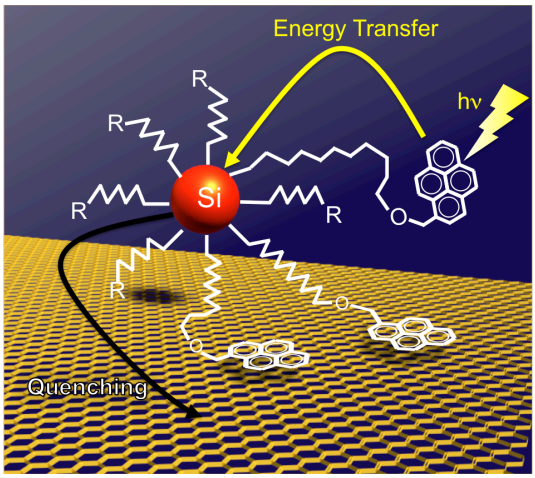

Figure 1: Schematized description of the photophysical interaction between Silicon Nanocrystals and Graphene

In the present study, hydride-terminated Si nanocrystals were used as a platform for co-passivation with dodecene and a pyrene derivative featuring a long alkyl chain and an alkene function at the terminal position by thermal hydrosilylation. Two different families of nanocrystals were studied with average diameter of 3 and 5 nm. Moreover, we studied the interaction and self-assembly of these functionalized nanocrystals with carbon-based

References

[1] Mastronardi, M. L. et al, *Adv. Mater.* **2012** , 24, 5890-5898
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materials of increasing complexity, from C60 to single-walled carbon nanotubes (SWCNTs) up to graphene [3].

The resulting material was characterized by transmission electron microscopy (Fig 2a) as well as solution phase and solid-state spectroscopic techniques (Fig 2b) to get information about the structure, morphology and the electronic interactions of the self-assembled structure. Further investigation of the graphene-SiNCs adducts was carried out by Kelvin Probe Microscopy experiments in order to get insights into the photogenerated charge transfer at the interface between the two materials.

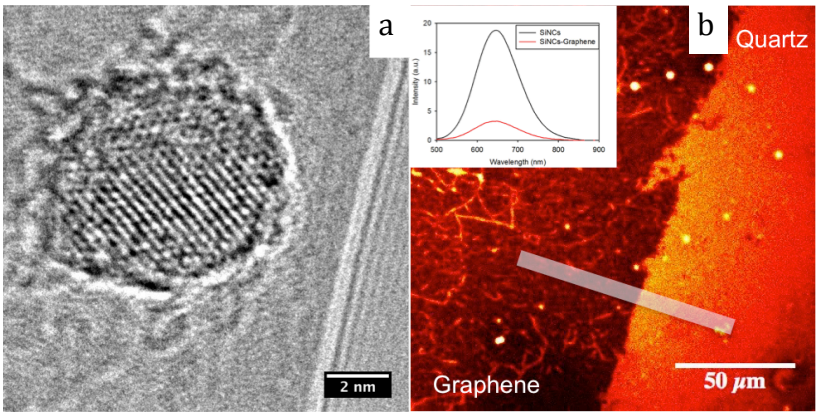

Fig. 1 a) HR-TEM micrograph of 6 nm SiNC on CVD graphene. b) Wide field Fluorescence micrograph of SiNCs deposited on graphene coated quartz and PL spectrum (inset)

The investigation of the interaction between the photoactive SiNCs and carbon allotropes opens the way to the application of such hybrid materials to many applications as photovoltaics, optoelectronics, as well as biosensors.