

Abstract Submitted
for the MAR15 Meeting of
The American Physical Society

Optical and electronic properties study of bottom-up graphene nanoribbons for photovoltaic applications¹ CESAR E.P. VILLEGAS, ALEXANDRE ROCHA, Instituto de Física Teórica, Universidade Estadual Paulista, São Paulo, SP, Brazil — Graphene nanoribbons (GNRs), turn out to be serious contender for several optoelectronic applications due to their physical properties. Recently, bottom-up methods, using the assembly of appropriate precursor molecules were shown to be an exciting pathway towards making precise nanoribbons. In particular, it has been demonstrated that so-called cove-shaped GNRs absorb light in the visible part of the spectrum, suggesting they could be used for photovoltaic applications. In solar cells, the key ingredient is the presence excitons and their subsequent diffusion along a donor material. This is influenced by the character of the different excitations taking place, as well as, the exciton binding energy. Thus, In this work we use many-body corrected density functional theory to simulate the optical properties of these nanoribbons. We elucidate the most important transitions occurring in these systems, and identify types of excitations that have not been previously observed in conventional nanoribbons. We also find that the exciton binding energies for all the structures we considered are in the eV range, which enhances the diffusion lengths for the particle-hole pairs. Finally, we estimate the potencial of these systems as solar cells by calculating the short-circuit current.

¹The Authors thank FAPESP for financial support

Cesar E.P. Villegas
Instituto de Física Teórica, Universidade Estadual Paulista,
São Paulo, SP, Brazil

Date submitted: 14 Nov 2014

Electronic form version 1.4