

# Width Dependent Charge Transport Modes in AGNR

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By means of a two dimensional tight-binding model with lattice relaxation in a first order expansion, we report different charge transport modes depending on the AGNR width family as well as on its size. We obtain that representatives of  $3p+2$  family do not present a polaronic mediated charge transport. As for  $3p$  and  $3p+1$  families, the polaron behavior was completely dependent on the system's width. Particularly, we observed a greater degree of delocalization for broader nanoribbons; narrower nanorribons of both families, on the other hand, typically presented a more localized polaronic-type transport. Energy levels and occupation numbers analysis are performed in order to rigourously assess the nature of the charge carrier. Time evolution in the scope of the Ehrenfest Molecular Dynamics was also carried out to confirm the collective behavior and stability of the carrier as a function of time. We were able to determine that polarons in nanoribbons of  $3p$  family present higher mobility than those in  $3p+1$  nanoribbons. These results are crucial to the correct evaluation of what kind of transport process takes place for each different system and also to predict the mobility of the charge carriers depending on structural properties of the system, so that they are expected to provide guidance for improving the efficiency of AGNRs based devices.