Graphene nanoribbons as low-bandgap donor materials for organic photovoltaic: Quantum-chemical aided design

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Graphene nanoribbons (GNRs) are strips of graphene cut along a specific direction with a nanometer sized width (< 10 nm). Compared to graphene, GNRs feature peculiar electronic and optical properties, such as the opening of a finite bandgap, which make them suitable for various applications in nanoelectronics and nanophotonics [1-8]. It is well known that the opto-electronic properties of GNRs can be tuned by changing their shape (from armchair to zigzag), periphery, widths and length [9-10]. As such, they are widely investigated for various applications in nanoelectronics and nanophotonics, namely as transparent electrodes in organic photovoltaic (OPV) cells. We show here by means of (time-dependent) density function theory calculations that GNRs with properly designed edge structures fulfill the requirements in terms of electronic level alignment with common acceptors (e.g., C_{60}) and solar light harvesting to be used as electron donors for OPV (considering the P3HT as refer donor), Figure 2. In addition, rearrangement of the electronic density at GNR-C_{60} interfaces strongly perturbs the energy diagram for electrons and holes favoring the splitting of the CT pairs into free charge carriers. Altogether, the electronic and optical properties of GNRs seem to be particularly well suited to ensure sunlight absorption and photoconvertion at interfaces with fullerenes in OPV devices.

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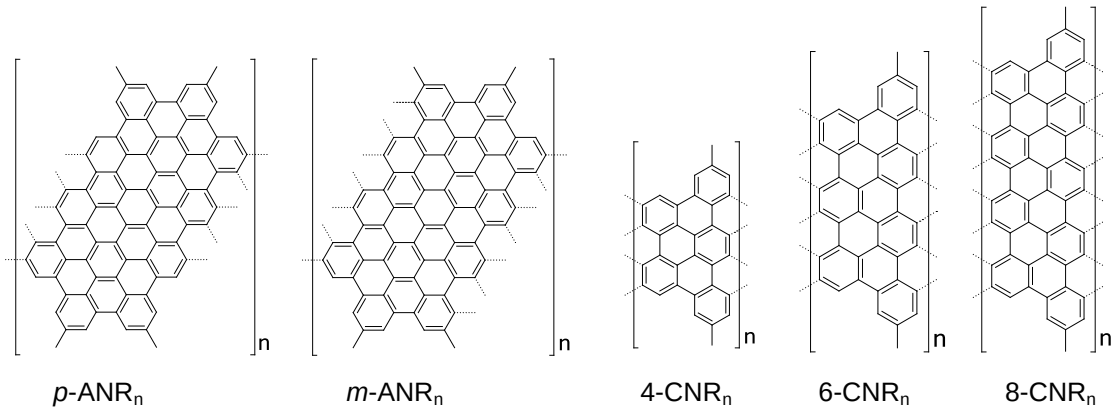

Figure 1. Chemical structures of the graphene nanoribbons investigated here. The n index is varying from 1 (monomer) to 4 (tetramer). *p*-ANR$_n$ and *m*-ANR$_n$ have the same repeating unit but differ by their connectivity (dashed lines). The difference in the CNR$_n$ series is due to the increase of the width in the sequence 4-CNR$_n$ < 6-CNR$_n$ < 8-CNR$_n$. For all structures, methyl group are used as side chains in the calculations.

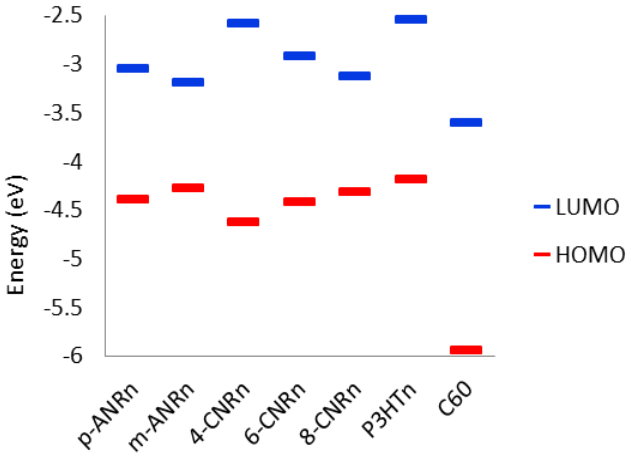

Figure 2. One-electron energy diagram for GNRs, P3HT (donors) and C_{60} (acceptor).