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Atypical structural, electronic, and thermoelectric properties of assembled graphene nanoribbons[1] LIANGBO LIANG, VINCENT MEUNIER, Rensselaer Polytechnic Institute, EDUARDO CRUZ-SILVA, University of Massachusetts, EDUARDO GIRÃO, Universidade Federal do Piauí — Highly ordered assembly of individual graphene nanoribbons (GNRs) into graphene nanowiggles (GNWs) has been recently demonstrated using a surface-assisted bottom-up chemical approach. GNWs are characterized by a periodic repetition of wiggle-like junctions where armchair- or zigzag-edged GNRs sectors alternate. We employed both density functional theory (DFT) and Tight-Binding+U to demonstrate their versatile electro-magnetic properties [Girão et al, Phys. Rev. Lett. 107 (2011)]. The coexistence of parallel and oblique sectors leads GNWs to offer a broader set of geometrical parameters to fine tune the electronic band gap from 0.0 eV to 1.7 eV than GNRs [Girão et al, Phys. Rev. B 85 (2012)]. Also, the presence of wiggle-like edges dramatically degrades thermal conductance but retains excellent electronic conduction, resulting in significant enhancement of the thermoelectric performance [Liang et al, Phys. Rev. B 86 (2012)]. Finally, many-electron GW calculations show quasiparticle band gaps of GNWs generally more than twice of their DFT band gaps, reaching 3.7 eV. Furthermore, the gold substrate where GNWs are synthesized is found to lead to band gap reduction owing to substrate polarization effect, consistent with experiments [Liang et al, Phys. Rev. B 86 (2012)].

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