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Electronic properties of graphene nanoribbons with multiple passivating edge species MARIA STOURNARA, VIVEK SHENOY, Brown University, ASHWIN RAMASUBRAMANIAM, University of Massachusetts — We suggest a novel approach of engineering the band gap of zigzag nanoribbons (ZGNRs) with multiple coexisting functional edge species, in particular, ZGNRs with varying ratios and spatial distribution of mixed oxygen and hydrogen passivation. Prior studies have already demonstrated that H-termination is responsible for semiconducting behavior of graphene, whereas O-termianation is purely metallic. Based on density functional studies, we show that ribbons with mixed O and H termination exhibit a rich variety of behavior that depends both upon the ratio of O and H atoms as well as their spatial distribution. In some instances it is even possible to double the band gap of H-terminated ZGNRs by introducing coexisting O edge atoms. We present a systematic analysis of these trends and propose a simple model to explain the observed behavior.

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