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**Engineering electronic properties of armchair graphene nanoribbons using strain and functional species** XIHONG PENG, FU TANG, SELINA VELASQUEZ, ANDREW COPPLE, Arizona State University — First principles density-functional theory calculations were performed to study effects of strain, edge passivation, and surface functional species on structural and electronic properties. Particularly band gap and work function, of armchair graphene nanoribbons (AGNRs), are addressed. It was found that the band gap of the O-passivated AGNRs experiences a direct-to-indirect transition with sufficient tensile strain. The indirect band gap reduces to zero with further increased strain. The work function was found to increase with uniaxial tensile strain while decreasing with compression. The variation of the work function under strain is primarily due to the shift of the Fermi energy with strain. For AGNRs with edge carbon atoms passivated by oxygen, the work function is higher than that of nanoribbons with edge passivated by hydrogen under a moderate strain. The difference between work functions in these two edge passivations is enlarged (reduced) under a sufficient tensile (compressive) strain. Furthermore, the effect of surface species decoration, such as H, F, or OH with different covering density, was investigated. It was found the work function varies with the type and coverage of surface functional species. F and OH decoration increase the work function while H decreases it. The surface functional species were decorated on either one side or both sides of AGNRs. The difference in the work functions between one-side and two-side decorations was found to be relatively small, which may suggest the introduced surface dipole plays a minor role.

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