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Tunable electronic properties of armchair graphene nanoribbons from first-principles calculations ANDREW COPPLE, XIHONG PENG, SELINA VELASQUEZ, FU TANG, Arizona State University — First principles density-functional theory calculations were carried out to study the effects of strain and edge passivation on electronic properties in armchair graphene nano-ribbons (AGNRs). We studied two types of strains (uniaxial expansion and compression) and five groups of edge passivation (H, F, OH group, bridged-O, and bridged-S). The investigated properties of the AGNRs include lattice constant, band gap, effective masses of charge carriers, and work function. We found strain and edge passivation play significant roles in modifying the electronic properties of AGNRs. Uniaxial strain effect on the energy gap shows a zig-zag pattern. Different edge passivation produces its unique zig-zag pattern due to their different optimized lattice constants. In the cases of bridged-O and bridged-S, a transition from direct to indirect band gap occurs at a sufficient tensile strain. With further increased tensile strain, the gap shrinks to zero. The work function increases with tensile strain and decreases with compression, regardless of the edge passivation. Such kinds of modulations of electronic properties in AGNRs are important for its applications in future electronics technology.

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