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Strain and edge passivation induced band gap modulation and effective mass tuning in Armchair Graphene Nanoribbons SELINA VELASQUEZ, PAUL LOGAN, XIHONG PENG, Arizona State University — We carried out a theoretical study of the effects of strains and molecular/chemical edge passivation on electronic properties in armchair graphene nano-ribbons (AGNR), using first principles calculations. The electronic properties we studied include band gaps and effective masses of the electron and hole. We found strain and edge passivation could significantly modify the gap and effective masses of AGNR. Three different patterns of strain-gap response, i.e., linear, concave and convex curves, are identified for different width of AGNR. Such kinds of modulations of electronic properties in AGNR are important for its applications in future electronics technology.

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