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Electron-phonon coupling effects in the (8-5-5) line defect of graphene nanoribbon HENG LUO, YONGWOO SHIN, XI LIN, Boston University — A "metallic" line defect in graphene nanoribbon consisting of alternating units of octagon and a pair of pentagons (8-5-5) is modeled using the adapted Su-Schrieffer-Heeger model Hamiltonian to include explicit electron-phonon coupling effects. Our results indicate that the 8-5-5 line defect has a finite optical gap of 0.4 eV with a broken charge conjugation symmetry, the bottom conduction band state mimic the nanoribbon edge case and the top valence state identical to the polyacetylene case. Upon photoexcitation, a small self-localized polaron state is found along one zigzag side of the line defect and a soliton-antisoliton pair is found on the other side. When the line defect is sandwiched between two graphene nanoribbons, the finite optical gap and photo-induced self-localized states persist as long as the nanoribbon width is smaller than 2 nm.

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