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Kohn anomalies and electron-phonon coupling in T-graphene M.E. CIFUENTES-QUINTAL, R. DE COSS, Departamento de Fisica Aplicada, Cinvestav-Merida — T-graphene is a metastable phase of graphene which consist in tetragonal rings of carbon atoms with a metallic behaviour. The Fermi surface of T-graphene consist of a hole pocket at the Γ point and a electron pocket at the M point, with large parallel portions which is expected to induce strong Kohn anomalies and a strong electron-phonon (e-ph) coupling. In this work, we present DFT first-principles calculations of the Kohn anomalies and electron-phonon coupling in T-graphene. Our calculations are based in the Plane-Waves and Pseudopotential method, with the GGA-PBE exchange-correlation functional. Dynamical matrices and e-ph coupling properties were computed with the linear response theory. We found a strong Kohn anomaly in two optical phonon branches at the M point, which consist in inter-band transitions from the two fermi surface pocket. The squared average of the electron-phonon coupling matrix elements at the Fermi surface of the Kohn anomalies are lower in comparison with the hexagonal ground-state graphene. The Eliashberg function, e-ph coupling constant, and the possibility of superconductivity are also analyzed.

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