Calculation of the superconducting transition temperature of a graphene layer doped with titanium and palladium. GERARDO VAZQUEZ, FERNANDO MAGANA, OSIRIS SALAS-TORRES, Instituto de Fisica, UNAM — We explore the structural interactions between graphene and transition metals such as palladium (Pd) and titanium (Ti) and the possibility of inducing superconductivity in a graphene sheet in two cases, one by doping its surface with palladium atoms sit on the center of the hexagons of the graphene layer and other by covering the graphene layer with two layers of titanium metal atoms. The results here were obtained from first-principles density functional theory in the local density approximation. The Quantum-Espresso package was used with norm conserving pseudopotentials. All of the structures considered were relaxed to their minimum energy configuration. Phonon frequencies were calculated using the linear-response technique on several phonon wave-vector mesh. The electron-phonon coupling parameter was calculated with several electron momentum k-mesh. The superconducting critical temperature was estimated using the Allen-Dynes formula with μ^* = 0.1 - 0.15. We note that palladium and titanium are good candidate materials to show a metal-to-superconductor transition. We thank Dirección General de Asuntos del Personal Académico de la Universidad Nacional Autónoma de México, partial financial support by Grant IN-106514 and we also thank Miztli Super-Computing center the technical assistance.

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