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**First principles studies of the interaction between metal clusters and graphene** RAISI BALDEZ, Universidade Federal de Santa Maria/Auburn University , PAULO PIQUINI, ALEX SCHMIDT , Universidade Federal de Santa Maria, MARCELO A KURODA, Auburn University — Due to its outstanding electrical, mechanical, and thermal properties, graphene is a promising material for a wide range of applications. However, making electrical contacts to this two-dimensional system has been a challenging task. In this work we analyze the interaction of small metal clusters with pristine and defective graphene layers using first principles calculations. The lowest energy structures of free clusters of different metals (Au, Pd, Pt and Ti) were obtained using a genetic algorithm approach. We find that the adhesion of these metal clusters in defective graphene, even if away from the defects, is substantially larger than in pristine graphene. Among the metals considered in our study, Ti clusters form the strongest binding with pristine or defective graphene. The resulting band structures show a strong hybridization of the Ti/C orbitals, which explains the origin of the enhanced binding energies.

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