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Analysis of the intercalation of oxygen at the Ru(0001)-Graphene interface[1] DANIEL TORRES, MARK HYBERTSEN, Brookhaven National Laboratory — The process whereby oxygen intercalates at the Ru(0001)-Graphene interface, resulting in systematic electronic decoupling of the graphene layer from the metallic substrate, depends on the interplay between graphene adhesion on the surface and the oxygen adsorption energy. We use density functional theory based calculations, including the effect of van der Waals interaction, to compare the energetics of competing phases in this process. We report three key findings. First, the van der Waals interaction makes a significant contribution to the binding of graphene to Ru(0001). Second, we assess the thermodynamic driving force between uniform oxygen phases on the clean surface and those intercalated at the interface. Third, we consider a series of local 1x1 oxygen patches centered on the raised region of the Ru(0001)-Graphene moiré which illustrate a series of stages in the decoupling of graphene from the Ru(0001) surface.

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