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Graphene on Ir(111) surface: interplay between chemical bonding and van der Waals PREDRAG LAZIC, NICOLAE ATODIRESEI, VASILE CACIUC, STEFAN BLUEGEL, Institut fuer Festkoerperforschung (IFF) and Institute for Advanced Simulation (IAS), Forschungszentrum Juelich, RADOVAN BRAKO, Rudjer Boskovic Institute, Zagreb, Croatia — Graphene is an interesting new material, which consists of carbon atoms forming a hexagonal lattice. Within graphene, carbon atoms are connected by strong chemical bonds but when graphene sheets bind to something else different binding mechanisms take place. For example, when graphene sheets bind among themselves forming graphite, bonding between them is exclusively of van der Waals type i.e. there is no formation of chemical bonds and sheets are only physisorbed one ontop of each other. A graphene sheet on top of Ir(111) surface is experimentally studied by means of STM and photoemission. In standard DFT calculations this system is not described correctly due to great importance of van der Waals binding. Employing the newly developed vdW-DF functional we have calculated this system and have shown that besides pure van der Waals binding additional chemical interaction takes place giving rise to interesting phenomena (anti-corrugation) to be observed in STM images.

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