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Ab-initio calculation of bonding, charge redistribution and transfer of graphene on amorphous silica NING SHEN, JORGE SOFO, Department of Physics, Penn State University — We study the effects of an amorphous silica substrate on the electronic structure and electron density of graphene using Density Functional Theory. We observe that the silica substrate transfers charge to the graphene layer and the workfunction of the combined system is lower than that of an isolated graphene sheet. The inhomogeneous charge distribution of the substrate induces an inhomogeneous charge redistribution on the graphene layer, which is experimentally observed as electron and hole puddles. The binding energy between one graphene layer and the substrate is weak and reveals no sign of chemical bonding. This can also be inferred from a rigid band shift observed in the system.

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