Oxynitride and Silicates at Epitaxial Graphene on SiC (0001)

HANSIKA SIRIKUMARA, JAIME BOHORQUEZ, THUSHARI JAYASEKERA, Southern Illinois University Carbondale — Epitaxial graphene, the sp²-hybridized network of carbon grown on another material is one way of creating large-scale graphene. Intercalated oxygen at the interface has shown to saturate the Si dangling bonds, and is a promising way of tuning the charge density in epitaxial graphene on SiC [1]. It would be interesting to investigate how oxy-nitrides and silicates at the SiC/graphene interface can change the electronic properties of the graphene layer.

Based on the first principles density functional theory calculations, we discuss the electronic and structural properties of epitaxial graphene on SiC with Si₂O₅ and SiON layers at the interface.