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Electronic properties of the Graphene/SiC (000$\bar{1}$) interface: a First Principles study THUSHARI JAYASEKERA, SHU XU, K.W. KIM, MARCO BUONGIORNO-NARDELLI, North Carolina State University — In this talk, we will discuss the electronic properties of epitaxial graphene on the SiC (000$\bar{1}$) surface (C-terminated face) using Density Functional Theory. In our calculations we focus on mono- and bi-layer graphene with AA, AB and turbostratic stacking sequences. Of the three, the turbostratic is the most observed during growth on SiC (000$\bar{1}$). However, no theoretical investigations are available to understand the effect of the substrate on this growth sequence. We will investigate the energetics of different stackings and explain their electronic properties. We will also discuss the role of the interfaces in the stabilization of the individual stacking sequences and indicate possible routes for chemical functionallizations at the heterojunction to facilitate the tuning of the electronic and transport properties of these systems.

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