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First principles-based moiré model for incommensurate graphene on BN[1] CATALIN SPATARU, KONRAD THURMER, Sandia National Labs — Various properties of supported graphene films depend strongly on the exact positions of carbon atoms with respect to the underlying substrate. While density functional theory (DFT) can predict atom position in many systems, it cannot be applied straightforwardly to systems that are incommensurate or have large unit cells, such as graphene on a BN surface. We address these limitations by developing a simple moiré model with parameters derived from DFT calculations for systems strained into commensurate structures with manageable unit cell sizes. Our moiré model, which takes into account the flexural rigidity of graphene and includes the influence of the substrate, is able to reproduce the DFT-relaxed carbon positions with an accuracy of <0.01 Å. We then apply this model to the unstrained C/BN system and predict how structure and energy vary with azimuthal orientation of the graphene sheet with respect to the BN substrate.

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