Abstract
We develop a multiscale continuum model to describe the interlayer defects in bilayer materials. The model incorporates both the anisotropy elasticity of each mono-layer in bilayer materials and the first-principle calculation informed interaction between two layers, i.e., the nonlinear atomistic potential energy between two layers. The equilibrium structures are obtained from the numerical simulations of the force balance differential equations. We apply this approach to determine the structure and energetics of twisted bilayer material. In tBLG, two distinct, modified Moiré structures are observed. Our model agrees well with the atomistic results. An analytical description is developed based on the obtained structural features.