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Edge-Edge interactions in stacked graphene EDUARDO CRUZ-SILVA, University of Massachusetts Amherst, XIAOTING JIA, Massachusetts Institute of Technology, MAURICIO TERRONES, The Pennsylvania State University, MILDRED DRESSELHAUS, Massachusetts Institute of Technology, VINCENT MEUNIER, Rensselaer Polytechnic Institute — Graphene is often considered as the ultimate material for nanoscale electronics due to its unique structure-dependent properties. It has recently been shown that edge reconstruction and reshaping using combined electron irradiation and Joule heating could be used to control graphene properties towards nanodevice design. For instance, HRTEM experiments on few-layered graphene have revealed the presence of small graphene patches and platelets over larger graphene domains. While these platelets usually move freely over the larger graphene surface, they sometimes get locked in positions close to the edges of the larger sheet, thereby modifying the local electronic environment. We modeled this behavior with extensive density functional calculations using the van der Waals functional of Dion et al. Local interactions at the edges are found to be sufficiently strong to explain the presence of stacking configurations (e.g. AA) that are known to be energetically unfavorable in 2D graphene. Our results explain the observed dynamics of these stacked platelets and provide a deeper understanding of graphene edge reconstruction.

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