Diffusion of Si and C atoms on and between graphene layers

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The growth of epitaxial graphene (EG) on the SiC substrate is accompanied by the evaporation of Si atoms during the growth process. The continuing loss of Si atoms takes place even after the surface graphene sheets have been formed. This atomic transport is believed to be a key element in establishing a growth mechanism to model and control the process. Using density functional theory (DFT) calculations, we have studied the diffusion of Si and C atoms on a single layer of graphene and between graphene sheets. The potential energy surfaces are explored. The research in this work would provide a detailed energetic description of relevant processes in the growth of epitaxial graphene.