Atomistic modeling of the directed-assembly of bimetallic Pt-Ru nanoclusters on Ru(0001)-supported monolayer graphene

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Abstract
The formation of Pt-Ru nanoclusters (NC’s) by sequential deposition of Pt and Ru on a periodically rumpled graphene sheet supported on Ru(0001) is analyzed by atomistic-level modeling and Kinetic Monte Carlo simulations. The periodic variation of the adsorption energy across the graphene sheet directs the assembly of NC’s to a periodic array of thermodynamically preferred locations. The modeling describes not just the NC densities and size distributions, but also the composition distribution for mixed NC’s. A strong dependence of these quantities on the deposition order is primarily related to different effective mobilities of Pt and Ru on the supported graphene.


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