GAPHENE NUCLEATION ONSET BY POLYCYCLIC AROMATIC HYDROCARBONS

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While graphene synthesis via chemical vapor deposition (CVD) with gaseous carbon precursors is extensively studied [1], the fundamental nucleation mechanisms involving polycyclic aromatic hydrocarbons (PAHs) are not fully elucidated. This research employs molecular dynamics (MD) simulations to analyze graphene nucleation from naphthalene and perylene deposited onto a Ni(111) surface. The simulations demonstrate that initial deposition triggers hydrogen dissociation and subsequent desorption, enabling the diffusion of dehydrogenated PAHs and the formation of a graphene layer (Figure 1). Analysis of the Gibbs free energy revealed that the transition from initial deposition to graphene formation resulted in a 0.3 eV decrease for naphthalene and a 0.6 eV decrease for perylene, signifying improved system stability.

**Figure 1.** The process of graphene nucleation from naphthalene (a → b) and perylene (c → d) molecules on the Ni(111) surface.



These findings contribute to a deeper understanding of PAH-driven graphene nucleation, offering potential for refined synthesis control.

REFERENCES

[1] Xiaoning Yang et al., Carbon **81** (2015): 564-573.