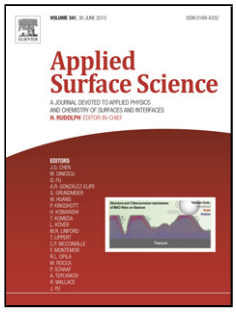

Title: Naphthalene Condensation as a Means of Producing Nanostructured Graphene

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Highlights:

- Interactions between arachic acid and naphthalene at the water surface have been simulated via AMBER force field model.
- The results of simulation are in agreement with compression isotherm data obtained via Langmuir-Blodgett method.
- Enthalpy and free Gibbs energy of catalytic naphthalene condensation into perylene were calculated using semiempirical (PM7) and DFT (B3LYP) methods.
- According to calculation results, Ni and Pd may be the most efficient catalysts for this reaction among the studied compounds.