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The rich landscape of organic molecules on graphitic surfaces: What molecular dynamics shows

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Nanometer–scale systems exhibit rich, interesting and novel behavior when adsorbed onto surfaces, in part because the species are confined and also because the adsorbate species interact more strongly than in the bulk. Organics such as pentacene, alkanes and fullerenes on graphene and graphite exhibit a wide variety of epitaxy, phases and phase transitions that are of fundamental scientific as well as technological importance. This presentation will provide an overview of molecular dynamics (MD) simulation techniques as well as mathematical characterization of the various phases and phase transitions realized by these fascinating systems.

Biography

Michael W Roth is a Computational Physicist and Professor and Chair at Northern Kentucky University's Department of Physics, Geology and Engineering Technology. He received a PhD in August 1992 and BS in Physics in May 1986 from Colorado State University. His research is on computational solid state physics. He has numerous publications and presentations in the field of dynamics and surface phase transitions of atomic and molecular systems adsorbed onto graphene and graphite. His other interests include classical astrophysical simulations of planetary formation as well as material point method simulations of impact and material stress and failure.

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