SEMINAR

Wednesday, 7th of March 2012 at 15:00

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Abstract

"Quantum Monte Carlo simulations of 4He clusters adsorbed on the surface of graphene."
Graphene, a single layer of graphite, which has demonstrated many surprising physical properties, is also of interest as a novel adsorber.
The talk will give an overview of our recent study of 4HeN clusters adsorbed on one and both sides of a graphene sheet. Different models for the interaction potentials will be discussed. We have modelled interactions of 4He clusters with graphene using an averaged helium-carbon potential that depends only on the distance to the graphene sheet, and a potential constructed as a sum of individual helium-carbon interactions. That way, we assess the effect of corrugation on the binding properties of helium clusters, both using isotropic and anisotropic interaction potentials. In addition, we asses the influence of the substrate mediated McLachlan interaction.
All the calculations have been performed using quantum Monte Carlo methods. At zero temperature the ground-state properties of 4HeN for 2â‰¤ Nâ‰¤100 have been determined using variational and diffusion Monte Carlo calculations. We find that clusters adsorbed on both sides of graphene are correlated. In addition, we observe the changes in the size of the clusters. For selected clusters, calculations have been performed also at finite temperature by path integral Monte Carlo simulations.