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Quantum Treatments for the Interaction of He Atoms with Carbon Layered Materials

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The interaction of He atoms with Polycyclic Aromatic Hydrocarbons (PAHS) or their extensions such as graphene, graphynes, and related carbon layered materials is a topic of interest in several areas that go from astrophysics to more fundamental research and technological applications.

For the study of these interactions is necessary to compute reliable potential energy surfaces (PES's) that can properly describe the short as well as the long range region. We have recently reported[1] a global PES for the interaction of He on the surface of the coronene, as well as that of graphene, that shows a good agreement with ab-initio estimations.

In this talk we will present some new results concerning the energetic and structure of small He_n@Coronene[2] clusters by means of Diffusion Monte Carlo (DMC) techniques.

The dynamics[3] of He atoms interacting with graphene and graphynes will be discussed based on our wave packet propagation code in full dimensions and within a reduced dimensionality model.

References

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[3] M. Bartolomei, E. Carmona-Novillo, M. I. Hernández, J. Phys. Chem. C, **118** 29966–29972 (2014)