Graphene-Based Nanocarriers: A Computational Study

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Open TASQ seminar

Friday Novemver 8th, 2024, 10.00 a.m. CEST,
Library of Faculty of Chemistry

In this talk, I will first introduce graphene and provide an overview of van der Waals aggregates and the role of dispersion forces in molecular systems then discuss ab initio electronic structure calculations, outlining standard computational techniques such as density functional theory (DFT) and their associated computational costs. The talk will also focus on the representation of the intermolecular potential using analytical formulae, applying these methods to increasingly complex molecular systems.

Finally, I will describe the computational methods used for the benchmarking of DFT functional for accurate simulations of large graphene prototypes. In addition, I will analyze the physical contributions to the total interaction energy, providing insights into the selection of appropriate functional for optimizing the performance of graphene as a nanocarrier.