Silica for drug-delivery: when simulation can complement experiment

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The delivery of drugs in the organism through nanocarriers is a topic of great interest in pharmaceutical research. An efficient Drug Delivery System (DDS) protects the drug from degradation, targets the diseased tissue and controls drug release. Among materials usually employed for drug delivery, silica plays a key role, particularly in its mesoporous form.

Although much research has been performed on the topic of silica drug delivery, the understanding of the interactions occurring between the material surface and drug molecules is still scarce, despite this knowledge is essential for determining the final performance of a DDS.

Molecular modeling can give a precious insight on this issue, acting as a "virtual microscope" to study the processes occurring inside the drug carrier. I will present here examples of how simulations can shed some light on silica-drug interactions and how their results can interface with and complement the experimental investigation, providing a collection of data (energetics, IR and NMR spectra, correlated to drug's feature and water content) that can help pharmaceutical researchers to better predict the features of novel drug delivery systems.