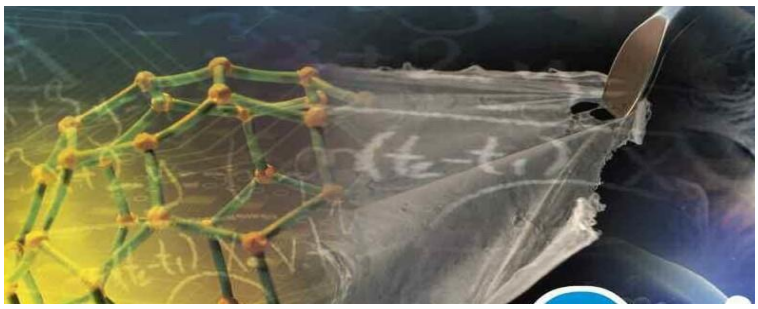
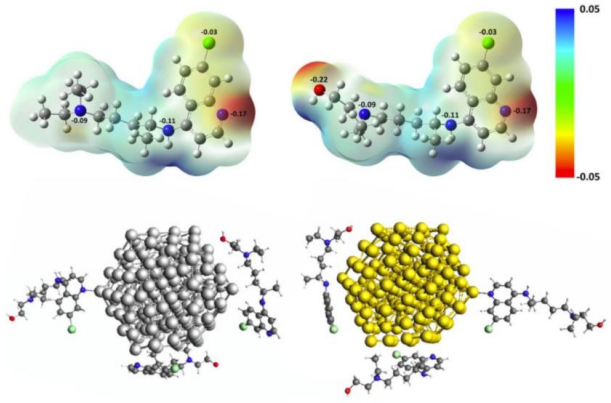


NANOSCIENCE & NANOTECHNOLOGY

Advancing knowledge through computer modelling



Charge distribution of HCQ and CQ molecules and their electrostatic potential map. Stable geometry of Ag_{147} and Au_{147} complexed with HCQ molecules (at BPE-D3/TZP level of theory).

Nanoparticles encapsulating drugs, or attaching to therapeutics, can be utilized as drug delivery systems to change drug biodistribution, decrease toxicity, modify drug release rate, and target affected tissues or cells. However, most nanoparticles are still in the clinical trial stage, with a few having been accepted for clinical use. In this regard, noble metal nanoparticles are well-known as promising materials that can transport drugs to specific targets in the body and be engineered to develop new delivery systems. Notably, silver, gold, and platinum nanoparticles reveal stability in the biological environment and survive in an intracellular environment.

The stable nanoparticles with small size possess the advantage of easily interacting with biomolecules both on the surface and inside cells, thereby playing a significant role in biomedical applications such as drug vehicles in diagnosing and treating diseases.

Given that the process of developing new drugs to become appropriate clinical candidates is extensive, one of the most rapid and reliable treatments is drug repurposing—the examination of existing FDA approved drugs for new therapeutic purposes. Chloroquine (CQ) and hydroxychloroquine (HCQ) have been used for many years as pharmacotherapies for malaria and were recently proposed as a potential therapeutic option against COVID-19. The pre-clinical studies have shown the prophylactic and antiviral effects of CQ and HCQ against SARS-CoV-2 (or COVID-19).

Current work is done under extended lockdown across the world, with no possibility of accessing experimental laboratories. In this situation, the work is just beginning for computational chemists and biophysicists to model the different approaches and propose efficient therapies to the experimentalists. Computational studies of molecular interactions of drugs can be used to develop the next-generation of drug inventions such as target-based drug discovery and delivery.

This paper has carried out the first principle density functional calculations to determine the affinity of HCQ/CQ molecules towards noble nanoparticles and confirm their weak interaction by theoretical UV–Vis absorption spectra. Our computational findings on the interaction of noble nanoparticles with drugs suggest these materials as potential vehicles for efficient HCQ/CQ usage to decrease their side efects.

This work was published by Razieh Morad, Mahmood Akbari, Parham Rezaee, Amin Koochaki, ***Malik Maaza*** *and Zahra Jamshidi as a Scientific Report.*

A full explanation of the research and its findings is available at link below:
https://www.nature.com/articles/s41598-021-81617-6