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**TiO<sub>2</sub> nanotubes as carriers for Cancer drugs (doxorubicin)****Fatemeh Mohammadpour***Farhangian university, Iran***Abstract**

**Statement of the Problem:** Doxorubicin (DOX) is a useful anthracycline chemotherapy agent derived from the *actinobacteria Streptomyces peucetius* var. *caesius* and is utilized to treat various cancers, including gastric, breast, thyroid, ovarian, lung, bladder, liver, sarcoma, and pediatric cancers. On the other hand, DOX can cause cardiotoxic effects forcing patients to discontinue treatment before eradicating cancer.

The purpose of this study is to encapsulate DOX into TiO<sub>2</sub> nanotubes to increase and improve the treatment efficiency of chemotherapeutics drugs and also address some problems of conventional therapeutic agents, including nonspecific distribution, poor solubility, and low therapeutic index.

**Methodology & Theoretical Orientation:** In this work, TiO<sub>2</sub> nanotubes were synthesized using a simple electrochemical anodization method, equipped with polyethylene caps and studied in view of their ability to

encapsulate and release the commonly used anticancer drug DOX. Drug loading into nanotubes was confirmed by Raman spectroscopy. Drug-release profiles were recorded by high-performance liquid chromatography (HPLC) under simulated physiological conditions. MD simulations were employed to investigate the interactions between DOX and a model TiO<sub>2</sub> nanotube at a molecular level, in particular, the loading of DOX.

**Conclusion & Significance:** steric bulk and pKa values (in bulk solution) probably results from the special confinement of DOX and water in the TiO<sub>2</sub> tubes. Summarizing the RDF and CDF calculations together with the calculated number of hydrogen bonds and their lifetimes confirms the good balance of the strength of the dominant DOX...water interactions with the "combined" forces of the DOX...DOX and DOX...TiO<sub>2</sub> hydrogen bonding interactions, in keeping with the initial simulation of the filling of the TiO<sub>2</sub> tube. Considering all together, our study shows why TiO<sub>2</sub> is competitive for the release of drugs of low polarity to the frequently used carbon or boron nitride (BN)-based materials.

**Biography**

Fatemeh Mohammadpour born in Isfahan, Iran, studied Physics at the University of Shiraz (M. Sc., 2009), and carried out her graduate studies "Optimization of TiO<sub>2</sub> and znO nanostructures to enhance conversion efficiency in dye-sensitized solar cells" (Ph. D. degree in 2014). From August 2013 to January 2014 she was guest scientist at the materials science faculty, LKO lab, at the Friedrich Alexander University of Germany where her research focused on application of TiO<sub>2</sub> nanotubes in dye-sensitized solar cells. She joined to the Zolghadr group at the chemistry faculty at the Shiraz University, Iran, in the post-doc position in the fall 2016 where her research focused on the use of nanoporous materials as drug carriers. Now she is assistant professor of physics at the Farhangian University, Shiraz, Iran from winter 2017

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