Computational modelling of pH Responsive Nanovalves in Controlled-release System.

Tomilola. J. Ajayi[†], Micheal. M Shapi[†]

[†]Department of Chemistry, Mangosuthu University of Technology, Durban 4031, KwaZulu-Natal, South Africa

ABSTRACT

A category of nanovalves system containing the cucurbit [7] uril ring on a stalk tethered to the pores of mesoporous silica nanoparticles (MSN) is theoretically and computationally modelled. This functions to control opening and blocking of the MSN pores for efficient targeted drug release system. Modelling of the nanovalves depend on the interaction between cucurbit [7] uril and the stalk in relation to pH variation. Protonation of the nitrogen atom on the stalk occur at acidic pH, leading to unsatisfactory host-guest interaction in the nanogate, hence there is dethreading. High required interaction energy and conformational change is theoretically established to drive the release of cucurbit [7] uril at a certain pH. The release was found to occur between pH 5-7 which agreed with reported experimental results.