Alternatives for Detection of Cs^+ by using Calix[4]arene-Crown-6

Girish Suravajhula and Pedro Derosa

Abstract

On the event of a calamity strike on nuclear power plant or a nuclear waste storage site, radioactive materials may spread into the environment and make it uninhabitable by humans. Cesium, the product of nuclear fission reaction is a primary component in high-level nuclear waste. Due to its high radioactivity and relatively long half-life Cs^+ is particularly dangerous and its detection and isolation from the environment is necessary for effective decontamination of the environment. 1,3-dimethoxycalix[4]arene-crown-6 (**I**) have been proven to be selective towards cesium and is currently used for its separation from nuclear wastes in the presence of other alkali metal ions. In this work three alternative designs for Cs^+ detection based on the 1,3-dimethoxycalix[4]arene-crown-6 molecule (The molecule), are studied by molecular simulation. In the first approach we considered the use of **I**-coated cantilevers, a maximum of ~680,000 molecules per μm^2 is predicted for efficient detection. In the second approach the change in the conductivity of 1,3-dimethoxycalis[4]arene-crown-6 after the absorption of the Cs^+ was considered as a possible alternative for sensing. Molecular orbital delocalization has been proved elsewhere to be associated with molecular conductivity. Frontier MOs are observed to delocalize across the calix[4]arene structure upon absorption of Cs^+. The final approach was to consider changes in molecular energy levels as an indication of the presence of Cs^+. The ionization potential of the molecule shows a change from 6.769 eV to 9.519 eV after the absorption of Cs^+, in general, all the energy levels around HOMO and LUMO show a stabilization. We predict that UV Photoelectron spectroscopy should show two peaks in the photoelectron energy spectrum, the one at low energy (larger binding energy) would be produced by molecules with Cs^+, while the peak at the higher energy (smaller binding energy), ~2.8 eV above the low energy peak, will indicate the presence of molecules with no Cs^+. An increase in intensity of the low energy peak will indicate the capturing of Cs^+.