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Construction of calixarene-based sensor: Multilayer Langmuir–Schaefer film and first-principles studies for 4-aminobenzoic acid sensing application

Abstract

Calixarenes, being well-known macrocyclic structures, have attracted considerable interest in the field of nanosensors due to their diverse advantages. 4-Aminobenzoic acid (PABA) was aimed to be detected by both calix[4]arene (C4) and calix[6]arene (C6) in this host-guest investigation. This study investigated the development of C4-PABA and C6-PABA complexes using the Langmuir–Schaefer (LS) method and first-principles density functional theory (DFT). All of the LS films formed were characterised by field emission scanning electron microscopy (FESEM), energy dispersive X-ray (EDX), carbon, hydrogen, nitrogen, oxygen elemental analyser (CHNS), ultraviolet-visible spectroscopy (UV-Vis), and Fourier-transform infrared spectroscopy (FTIR). Additionally, this work applied DFT to compute the binding energy and band gap. Morphological and elemental analysis based on the conducted characterisations indicated the incorporation of PABA via lower rims into both C4 and C6. The computed binding energy and band gap validated the experiment's findings that promising reactivity existed between calixarenes and PABA with the formation of stable complexes. The sensing of PABA by both C4 and C6 was proven. In the near future, the outcomes of this research can be applied to drug delivery systems for pharmaceutical and medical purposes.

Keywords

Calixarenes; Density functional theory; Host-guest; Langmuir–Schaefer; PABA; Sensor