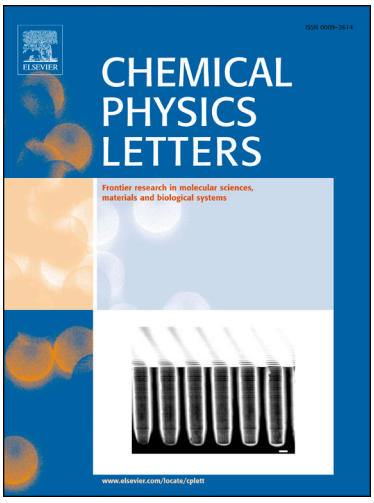


Research paper

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# Theory after experiment on sensing mechanism of a newly developed sensor molecule: Converging or diverging?

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## Abstract

Fluoride ion sensing mechanism of 3,3'-bis(indolyl)-4-chlorophenylmethane has been analyzed with density functional and time-dependent density functional theories. Extensive theoretical calculations on molecular geometry & energy, charge distribution, orbital energies & electronic distribution, minima on potential energy surface confirmed strong hydrogen bonded sensor-anion complex with incomplete proton transfer in $S_0$. In $S_1$, strong hydrogen bonding extended towards complete ESDPT. The distinct and single minima on the PES of the sensor-anion complex for both ground and first singlet excited states confirmed the concerted proton transfer mechanism. Present study well reproduced the experimental spectroscopic data and provided ESDPT as probable fluoride sensing mechanism.

## Introduction

In order to accelerate the incorporation of emerging sensor materials for new applications and to regulate the efficiency of a sensor, it is immensely important to know the exact functioning mechanism of the sensor molecule. Proper understanding of the sensing mechanism may develop ideas about the controlling factors that govern the sensing ability. Also, by monitoring the key factors, synthetic chemists can monitor the sensor efficacy to detect any ion instantly without any intricate technique. A number of theoretical mechanism explorations basically by using density functional theory (DFT) [1-5] motivated us to perform our present assay. Keeping all these in mind, we investigated and developed the mechanism behind sensing of an excellent fluoride ion sensor experimentally reported in recent past [6].