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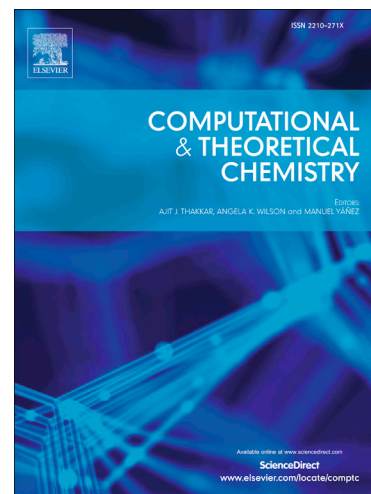
Theoretical research on the effect of Eosin Y adsorption action on Ru<sub>4</sub> and Pt<sub>4</sub> clusters on the hydrogen evolution performance

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# Theoretical research on the effect of Eosin Y adsorption action on Ru<sub>4</sub> and Pt<sub>4</sub> clusters on the hydrogen evolution performance

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**Abstract:** This work investigated the adsorption of Eosin Y (EY) on the surface of Ru<sub>4</sub> and Pt<sub>4</sub> clusters and the UV-vis adsorption of EY by the DFT and TD-DFT method, respectively. The relationship of adsorption action, adsorption energy and hydrogen production efficiency in EY-sensitized system were studied as well. It is proved that the enhancement in the interaction energy of key group in sensitizer and co-catalyst was an efficient method to improve hydrogen evolution performance. The TD-DFT calculation showed that the photoelectrons of excited state EY mainly focused on the upper surface of C<sub>5</sub>O ring with the COO<sup>-</sup> side. In the EY-Ru<sub>4</sub> system, the maximum adsorption energy originated from the concurrent interaction of the COO<sup>-</sup> and C<sub>5</sub>O groups of EY with the Ru<sub>4</sub> cluster was -237.8 kJ/mol, while in the EY-Pt<sub>4</sub> system the maximum adsorption energy from the interaction between the C atom on C<sub>6</sub> ring of EY and the Pt<sub>4</sub> cluster was -230.5 kJ/mol. Compared with EY-Pt system, the dominating adsorption of EY on Ru was conducive to the quick transfer of photoelectron from EY to Ru. Therefore, the EY-Ru system exhibited higher hydrogen generation efficiency than the EY-Pt system.

**Keywords:** Eosin Y, Ru<sub>4</sub>, Pt<sub>4</sub>, DFT, Adsorption energy, Hydrogen evolution performance.

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