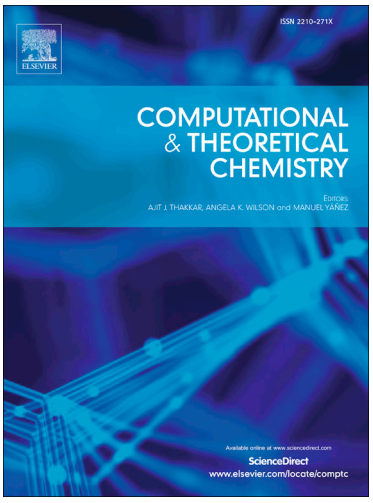

Theoretical research on the effect of Eosin Y adsorption action on Ru_4 and Pt_4 clusters on the hydrogen evolution performance

Yan-Xia Han, Chao Kong, Li-Jie Hou, Bo-Wan Wu, Qi Zhang, Zhi-Yuan Geng

PII: S2210-271X(18)30496-1
DOI: https://doi.org/10.1016/j.comptc.2018.08.019
Reference: COMPTC 12334

To appear in: *Computational & Theoretical Chemistry*

Received Date: 21 April 2018
Revised Date: 28 August 2018
Accepted Date: 28 August 2018

Please cite this article as: Y-X. Han, C. Kong, L-J. Hou, B-W. Wu, Q. Zhang, Z-Y. Geng, Theoretical research on the effect of Eosin Y adsorption action on Ru_4 and Pt_4 clusters on the hydrogen evolution performance, *Computational & Theoretical Chemistry* (2018), doi: https://doi.org/10.1016/j.comptc.2018.08.019

Theoretical research on the effect of Eosin Y adsorption action on Ru_4 and Pt_4 clusters on the hydrogen evolution performance

Yan-Xia Han[a,b] Chao Kong[b] Li-Jie Hou[b] Bo-Wan Wu[b] Qi Zhang[b] Zhi-Yuan Geng[a*]

(*[a]College of Chemistry and Chemical Engineering, Northwest Normal University, Lanzhou 730070*)

(*[b]College of Chemistry and Chemical Engineering, Longdong University, Qingyang Gansu 745000)*

Abstract: This work investigated the adsorption of Eosin Y (EY) on the surface of Ru_4 and Pt_4 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_5O ring with the COO^- side. In the EY-Ru_4 system, the maximum adsorption energy originated from the concurrent interaction of the COO^- and C_5O groups of EY with the Ru_4 cluster was -237.8 kJ/mol, while in the EY-Pt_4 system the maximum adsorption energy from the interaction between the C atom on C_6 ring of EY and the Pt_4 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_4, Pt_4, DFT, Adsorption energy, Hydrogen evolution performance.