MINISTRY OF EDUCATION AND TRAINING
QUY NHON UNIVERSITY

SOCIALIST REPUBLIC OF VIETNAM
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INFORMATION
ON THE NEW CONTRIBUTIONS OF DOCTORAL THESIS

(Information will be posted on the Website)

Title: *Study on adsorption ability of some organic compounds on TiO_2 and clay minerals materials by using computational chemistry*

Speciality: Theoretical and Physical Chemistry Code No.: 9440119

PhD student: Nguyen Ngoc Tri

Course: 4 (2016 - 2020)

Advisors: Assoc.Prof. Nguyen Tien Trung (Quy Nhon University), Prof. Minh Tho Nguyen (KU Leuven, Belgium)

Training institution: **Quy Nhon University**

NEW CONTRIBUTIONS OF THE THESIS

1/ The results of the thesis provide us an insight into the adsorption of organic molecules, antibiotics containing different functional groups such as -OH, -COOH, -CHO, >C=O, NO_2, $-NH_2$, $-SO_3H$ on the material surfaces including TiO_2 and clay minerals.

2/ The achieved results in this work give a good assessment of the adsorption processes that take place on the surfaces of TiO_2 and clay minerals. This is an important investigation for guiding subsequent experimental studies to remove or decompose pollutants in wastewaters.

3/ The role and origin of intermolecular interactions contributing to the stability of configurations as well as the adsorption capacity of molecules on the TiO_2 and clay mineral surfaces are clarified by using quantum chemical methods.

Binh Dinh, May 31st 2021

Advisors

Assoc.Prof. Nguyen Tien Trung

PhD student

Nguyen Ngoc Tri