

Hexu Ye

Master

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EXPERIENCE

Undergraduate

Qingdao University, China

2014/9-2018/6

Qingdao, Shandong province, China

Master

Shanghai University, China

2018/9-Ongoing

Shanghai, China

PROJECTS

Project 1:

A rotational study of O-H... π Hydrogen Bond: Styrene-water as a case.

- Experimental evidence irrefutably shows that water links to styrene through one O-H... π benzene hydrogen bond creating entgegen and zusammen configurations with respect to the vinyl group. The configuration and geometry of the observed isomer provide opportunity to benchmark quantum mechanical calculations.

Project 2:

A systematic search for the best methods to describe disulfide bond.

- The disulfide bonds, including covalent disulfide bond and weak electrostatic interactions are important structural features in astronomy, biology and many fields of chemistry. Here, density functional theory (DFT) methods with and without dispersion corrections, couple-cluster methods and empirical methods are applied to investigate model systems with disulfide bond. The focus is on accuracy of structural parameters, considering best available theoretical and experimental results as a reference.

MY LIFE PHILOSOPHY

"Imagination is more important than knowledge. For knowledge is limited, whereas imagination embraces the entire world, stimulating progress, giving birth to evolution.

—Albert Einstein"

STRENGTHS

Hard-working

Eye for detail

Creatively&curious

Python

Cfour

GAUSSIAN

Statistical Analysis

LaTex

