

Materials List for:

# Isotopic Effect in Double Proton Transfer Process of Porphycene Investigated by Enhanced QM/MM Method

Zhihui Tu<sup>1,2</sup>, Jian Yin<sup>3</sup>, Liangxu Xie<sup>4</sup>

<sup>1</sup>State Key Laboratory of Structural Chemistry, Fujian Institute of Research on the Structure of Matter, Chinese Academy of Sciences

<sup>2</sup>University of Chinese Academy of Sciences

<sup>3</sup>XtalPi Inc. (Shenzhen Jingtai Technology Co., Ltd.)

<sup>4</sup>Institute of Bioinformatics and Medical Engineering, School of Electrical and Information Engineering, Jiangsu University of Technology

Correspondence to: Liangxu Xie at [xieliangxu@jsut.edu.cn](mailto:xieliangxu@jsut.edu.cn)

URL: <https://www.jove.com/video/60040>

DOI: [doi:10.3791/60040](https://doi.org/10.3791/60040)

## Materials

Name	Company	Catalog Number	Comments
operating system	CentOS Linux release 6.0		
QM4D software	<a href="http://www.qm4d.info/">http://www.qm4d.info/</a>		in-house program
Computer desktop	HP		