

### Keggin型 $\alpha$ - $[\text{H}_x\text{W}_{12}\text{O}_{40}]^{(8-x)-}$ ( $x=1\sim 4$ )中心质子数及笼腔内外质子传递的DFT研究

王金月<sup>①</sup>, 蒲岚<sup>①</sup>, 罗华锋<sup>①</sup>, 胡常伟<sup>②</sup>, 熊燕<sup>③</sup>, 谭超<sup>①</sup>, 吴同<sup>①</sup>, 王健<sup>①</sup>, 王藩侯<sup>①</sup>

① 宜宾学院计算物理四川省高等学校重点实验室, 应用化学研究所, 宜宾 644007;

② 四川大学化学学院绿色化学与技术教育部重点实验室, 成都 610064;

③ 重庆大学化学化工学院, 重庆 400044

### DFT investigation on the internal proton numbers and their transfer throughout the cage of the Keggin-type $\alpha$ - $[\text{H}_x\text{W}_{12}\text{O}_{40}]^{(8-x)-}$ ( $x=1\sim 4$ )

WANG JinYue<sup>1</sup>, PU Lan<sup>1</sup>, LUO HuaFeng<sup>1</sup>, HU ChangWei<sup>2</sup>, XIONG Yan<sup>3</sup>, TAN Chao<sup>1</sup>, WU Tong<sup>1</sup>, WANG Jian<sup>1</sup>, WANG FanHou<sup>1</sup>

1. Key Laboratory of Computational Physics in Universities of Sichuan Province, Institute of Applied Chemistry, Yibin University, Yibin 644007, China;

2. Key Laboratory of Green Chemistry and Technology of Ministry of Education, College of Chemistry, Sichuan University, Chengdu 610064, China;

3. School of Chemistry and Chemical Engineering, Chongqing University, Chongqing 400044, China

[摘要](#)[图/表](#)[参考文献\(0\)](#)[相关文章\(6\)](#)[点击分布统计](#)[下载分布统计](#)