

Adsorption and infrared analysis of acrylic acid over Mo₂C

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Synopsis: Adsorption and infrared analysis of diferents acrylic acid structures over orthorrombic Mo₂C for corroborate with global mechanism and experimental data interpretation.

INTRODUCTION

Noble metal catalyst (platinum and palladium, for example) could be substituted by cheaper transition metal carbides. Molybdenum carbide (Mo₂C) was recently used for a several reactions with Pt-like catalytic behavior, high activity and selectivity and CO and sulfur compounds poisoning resistance. Molybdenum carbide was used for hydrogenation, decomposition and hydrodeoxygenation (HDO) reactions [1].

It's not clear how HDO reaction over Mo₂C occur in fatty acids formed by thermal cracking of triglycerides in bio-oil and biomass because there is only a few microscopy experimental evidences of this system [2]. For clarifying this, acrylic acid adsorption structures and normal modes was obtained in a DFT level over orthorhombic Mo₂C (001) for corroborate with global mechanism and experimental data interpretation. This molecule is a prototype for fatty acid because possesses the minimal structural features.

METHODS

All calculation was made at DFT level with Generalized Gradient Approximation (GGA) functional PBE with periodic boundary condition (PBC). The energy cutoff for plane wave basis set was 410 eV.

Self-consistent field (SCF), geometry optimization and phonons calculations were done in the projector augmented wave (PAW) approximation in Vienna Ab-Initio Simulation Package (VASP).

RESULTS AND DISCUSSION

Protonated and deprotonated acrylic acid structures were studied in different conformations, orthogonal and parallel adsorption structures.

For all structures, deprotonated always have lower adsorption energy because in this case there are more bonds between adsorbate and surface, one more oxygen-molybdenum bound. Comparing orthogonal and parallel structures, the first ones has

overall lower adsorption energies because in this case there are two bonds between surface and molecule, by carbonyl group and carbon in double bound. The lower adsorption energies are in table 1. Orthogonal (a) and parallel (b) deprotonated structures 4 are in figure 1. Phonon calculations of all structures are in progress.

Table 1. Lower adsorption energies

# Structure	Specie	Type	Adsorption Energy (Kcal/mol)
1	Acid	Orthogonal	-30
1	Acid	Parallel	-55
2	Acid	Orthogonal	-23
2	Acid	Parallel	-71
4	Acid	Orthogonal	-28
4	Acid	Parallel	-62
1	Deprotonated	Orthogonal	-53
1	Deprotonated	Parallel	-84
2	Deprotonated	Orthogonal	-76
2	Deprotonated	Parallel	-91
4	Deprotonated	Orthogonal	-80
4	Deprotonated	Parallel	-91

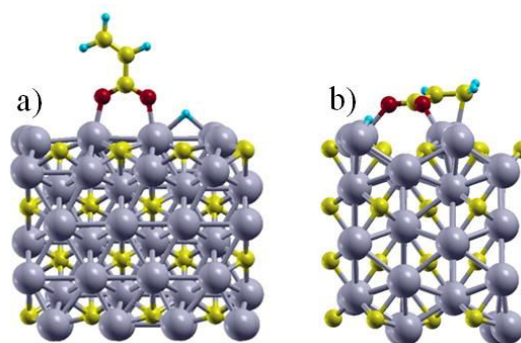


Figure 1. Orthogonal (a) and parallel (b) deprotonated structures 4

REFERENCES

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