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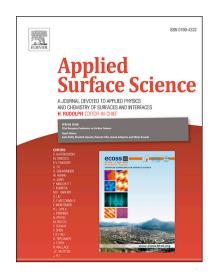
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ACCEPTED MANUSCRIPT

Dissociation mechanisms of HFO-1336mzz(Z) on Cu(1 1 1), Cu(1 1 0) and Cu(1 0 0) surfaces: A density functional theory study

Erguang Huo¹, Chao Liu^{1*}, Xiaoxiao Xu¹, Qibin Li², Chaobin Dang ³

- 1. Key laboratory of low-grade Energy Utilization Technologies and Systems, Ministry of Education, College of
 - Power Engineering, Chongqing University, Chongqing 400030, China
 - 2. College of Aerospace Engineering, Chongqing University, Chongqing 400030, China
- 3. Department of Human and Engineered Environmental Studies, The University of Tokyo, 5-1-5 Kashiwanoha,

Kashiwa-shi, Chiba 277-8563, Japan

*Corresponding author: Chao Liu. Tel: +86 023 65112469; fax: +86 023 65112469

E-mail address: <u>liuchao@cqu.edu.cn</u>

Abstract: The catalytic effect of Cu(1 1 1), Cu(1 1 0) and Cu(1 0 0) surfaces on the HFO-1336mzz(Z)decomposition of have been investigated by using Density Functional Theory (DFT) calculations. On the basis of adsorption energy analysis, the most stable adsorption energies of HFO-1336mzz(Z) and relevant products on Cu(1 1 1), Cu(1 1 0) and Cu(1 0 0) surfaces were studied, respectively, and the co-adsorption structures of relevant species were obtained. Finally, four initiation decomposition reactions of HFO-1336mzz(Z) on Cu(1 1 1), Cu(1 1 0) and Cu(1 0 0) surfaces were proposed and investigated, respectively. At the same time, the four similar homolytic reactions of free HFO-1336mzz(Z) molecular were calculated to compare with the dissociation reactions occurred on Cu(1 1 1), Cu(1 1 0) and Cu(1 0 0) surfaces and illuminate the catalytic effect of Cu(1 1 1), Cu(1 1 0) and Cu(1 0 0) surfaces on the HFO-1336mzz(Z) decomposition. The results indicated that Cu(1 1 1), Cu(1 1 0) and Cu(1 0 0) surfaces had a good catalytic effect on the decomposition of HFO-1336mzz(Z). The fracture reactions of C=C bonds on Cu(1 1 1), Cu(1 1 0) and Cu(1 0 0) surfaces were easier to occur than that of other reactions. Cu(1 0 0) surface had the highest catalytic activity and the lowest for Cu(1 1 1) surface.

Key words: Catalytic; Decomposition; HFO-1336mzz(Z); Density Functional Theory (DFT); Cu surface;

1. Introduction

Organic Rankine Cycle (ORC) is a promising approach for the recovery of the waste heat

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