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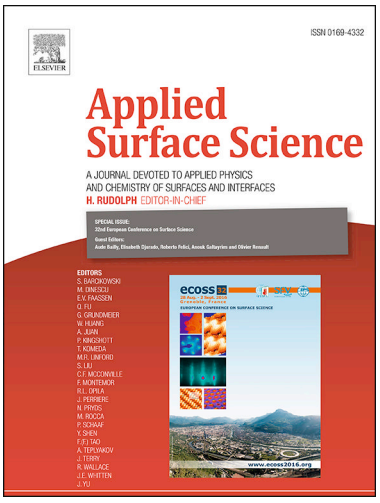


Full Length Article

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# 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

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**Abstract:** The catalytic effect of Cu(1 1 1), Cu(1 1 0) and Cu(1 0 0) surfaces on the decomposition of HFO-1336mzz(Z) 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