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Erratum

Erratum to "Selectivity driven design of bimetallic ethylene epoxidation catalysts from first principles" [J. Catal. 224 (2004) 489–493] ☆

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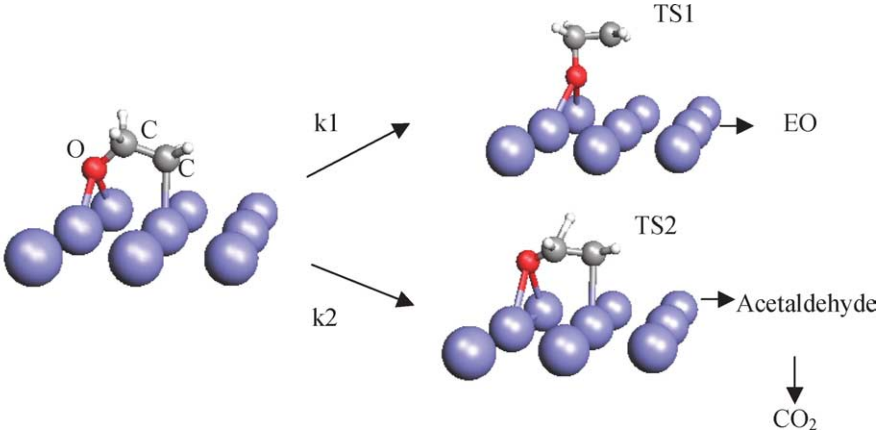
The publisher regrets that Figs. 1 and 2 did not reproduce well in the print issue. For the reader's convenience, the figures are reproduced here along with their legends.



(a)

Fig. 1. (a) Schematic of the reaction coordinates for competing oxametallacycle reaction pathways calculated using the NEB (Nudged Elastic Band) algorithm [14,15]. The formation of EO is characterized by C–O ring closure, while acetaldehyde is formed via a 1,2-H shift from the central to the terminal C atom. Activation barriers for both processes are calculated to be approximately 17 kcal/mol. The surface is the close packed Ag(111) surface. (b) Structure of bimetallic model catalysts investigated in high-throughput computational screening. There is one adsorbate, the surface oxametallacycle, or one transition state per unit cell. The atoms labeled B, C, and D in the unit cell are Ag atoms while A represents an impurity element. (c) The results of the computational screening; $\Delta\Delta E_A$ is calculated as a function of catalyst composition. The higher energy difference means that the bimetallic is predicted to be a more selective catalyst than monometallic silver.

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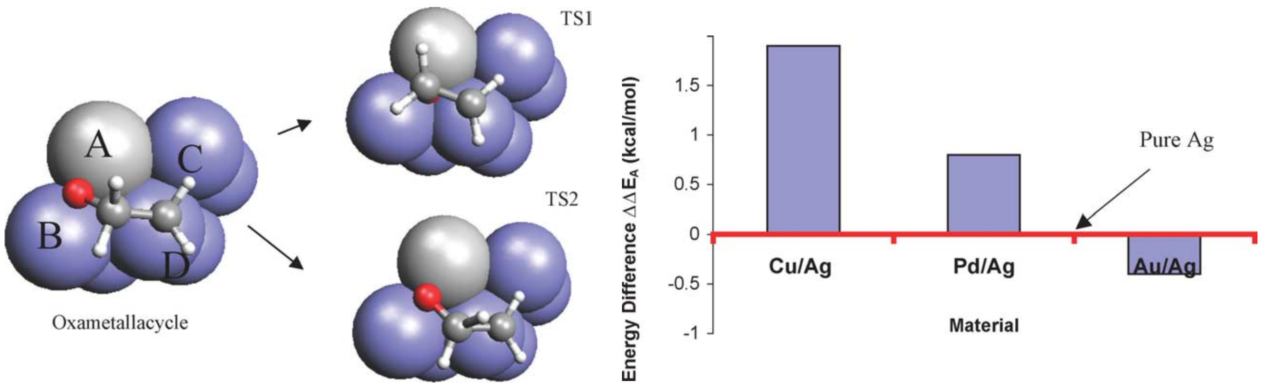

(b) (c)

Fig. 1. Continued.

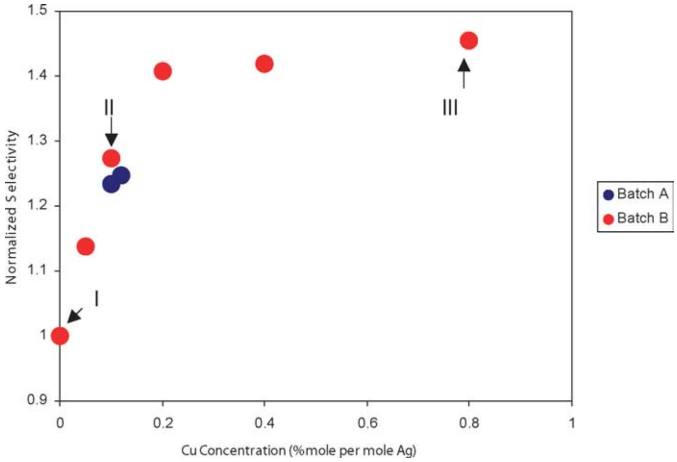

Fig. 2. Normalized catalyst selectivities to EO, i.e., the measured selectivity divided by the selectivity of pure Ag under the same conditions as a function of bulk Cu content. For catalysts labeled I, II, and III we have performed XPS studies to measure the amount of Cu in the top layers of a catalyst. For catalyst I there is no Cu present, catalyst II has ∼ 9 Cu atoms per 100 surface metal atoms, while catalyst III has ∼ 43 Cu per 100 Cu + Ag atoms in the surface layers. It is observed that Cu is enriched at the surface, as predicted.