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Symposium Title: (CATL002) Molecular Insights Towards Novel Catalysts

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Reason for Abstract Submission: I am contributing this paper in response to the Call for Papers.

Invitation from: No response indicated

Email of Inviter: No response indicated

Criteria are met: Are met by at least one author

Presenting author will register: Yes

Abstract will be withdrawn if author cannot attend: Yes, I agree

Abstract submitted only once: Yes, I agree

Equipment Needs: No response indicated

Comments to Organizers: No response indicated

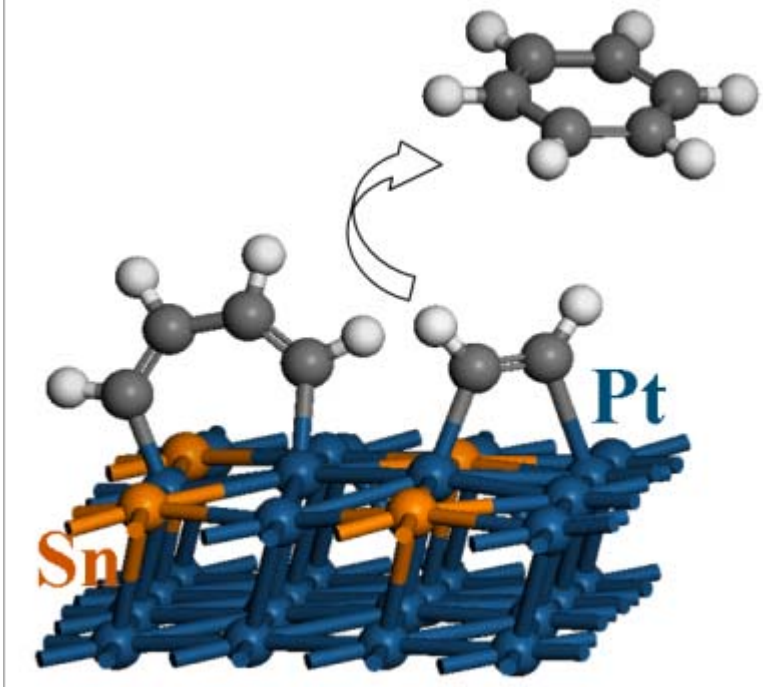
Preferred Presentation Method: Oral Preferred

Should this Paper be Considered for a SCI-MIX? No response indicated

Student Type: No response indicated

Title: Experimental spectroscopic and computational DFT studies of the mechanism of acetylene conversion to benzene on Pt-Sn alloys

Abstract Body: Conversion of regular and deuterated acetylene into benzene was studied on Pt(111) and two ordered surface alloys: Pt_3Sn/Pt(111) and Pt_2Sn/Pt(111) with HREELS and TPD at 90-1000 K. No benzene formation was detected on Pt(111). On alloys, formed benzene readily desorbs, and the amount of produced benzene is higher over the Pt_2Sn alloy with a higher Sn concentration. DFT calculations were performed in order to assign experimental vibrational frequencies and develop a molecular reaction mechanism for benzene formation. The results suggest that acetylene forms a cyclic C_4H_4 dimer on the Pt-Sn alloys. This C_4H_4 intermediate is predicted to produce benzene by reacting with an additional surface acetylene. The destabilizing effect of Sn alloying is more significant for acetylene than for the C_4H_4 intermediate, and as a result, the reaction of C_4H_4 formation changes from being endothermic on pure Pt to being exothermic, *i.e.* energetically favorable, on the Pt-Sn alloys.



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