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Symposium Title: (COMPenvSusSol01) Applications of Computational Methods to Environmentally Sustainable Solutions

INSTITUTIONS

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Reason for Abstract Submission: I was specifically invited to submit this paper.

Invitation from: George Fitzgerald

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Abstract will be withdrawn if author cannot attend: Yes, I agree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

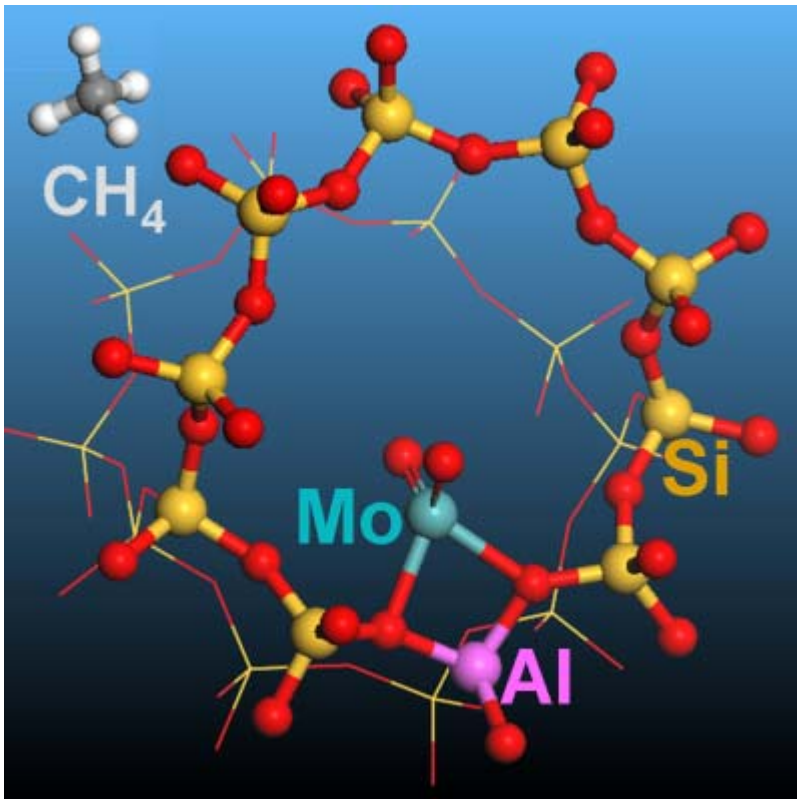
Preferred Presentation Method: Oral Preferred

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

Student Type: No response indicated

Title: Identification of catalytic molybdenum nanostructures on ZSM-5 for natural gas processing based on DFT calculations and operando molecular spectroscopy

Abstract Body: Methane conversion into valuable aromatic products represents a highly desirable route for conversion of natural gas into liquid fuels and chemical feedstocks. An integrated computational-experimental study was performed for identifying catalytic molybdenum nanostructures supported on ZSM-5 that convert methane into liquid aromatic hydrocarbons. Information from *operando* Raman and UV-vis spectroscopy and from simultaneous online mass spectrometer analyses was successfully consolidated with DFT calculations.



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