

Abstract Submitted  
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**First-principles investigations for the catalytic dissociation and oxidation of methane on the Cu surfaces**<sup>1</sup> YING LI, JAGAN MAHADEVAN, SANWU WANG, The University of Tulsa — The catalytic reactions of dissociation and oxidation of methane on the copper surfaces play a key role in, for example, the development of high-performance solid oxide fuel cells. We used first-principles quantum theory and large-scale parallel calculations to investigate the atomic-scale mechanism of the catalytic chemical reactions. We report the calculated results, which provide fundamental information and understanding about the atomic-scale dynamics and electronic structures pertinent to the reactions and specifically the catalytic role of the Cu(100) and Cu(111) surfaces. We also report comparison of our results with available experimental data and previous theoretical investigations.

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Sanwu Wang  
The University of Tulsa

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