The Reaction of Methane with Platinum Oxide Nanoclusters: A Computational Study

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Previous studies have shown that small clusters of transition metals like Pt, when reacted with oxygen, have useful catalytic properties compared to thin-film or bulk catalysts. These clusters have the potential for use in developing cheaper methods for converting propane to propene, which is a high-value compound used in making plastics. Understanding the structure and formation of these clusters is essential to gauging how reactive each catalyst is. Computational studies of Pt4O2 are being done using Gaussian 03 to understand their formation, and determine the stability of different spin states. The effectiveness of these clusters is then being tested using methane as a simple test molecule. The pathways for the Pt4 + O2 reaction, including transition state structures, for both singlet and triplet spin states have been identified, and the final products are currently being tested for reactivity using the methane molecule.

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