

Abstract Submitted  
for the MAR12 Meeting of  
The American Physical Society

**The role of non-conventional supports for single-atom  
Platinum-based catalysts in fuel cell technology: A theoretical  
surface science approach** ALOYSIUS SOON, RENQIN ZHANG,

Yonsei University, Seoul, Korea — Platinum-based heterogeneous catalysts are known to play a key role in the fuel cell technology, such as their use in the low-temperature proton exchange membrane (PEM) fuel cells. However, the high cost and low lifecycle of these PEM fuel cells are the major hindrances to its large-scale commercial production. To elevate the high-cost and to optimize its catalytic activity, it was recently proposed that catalysts with single-Pt atom dispersions and a more durable, corrosion-resistant TiN support could play an important role in the next generation of Pt-based PEM fuel cells [1]. As a first step towards a microscopic understanding of single-Pt atom-dispersed catalysts on these new supports, we present density-functional theory (DFT) calculations to investigate the adsorption properties of Pt atoms on pristine TiN(001). Optimized atomic geometries, energetics, and analysis of the electronic structure of the Pt/TiN system are reported for various surface coverages of Pt. We find that atomic Pt does not bind preferably to the clean TiN surface, but under operational conditions, TiN surface vacancies play a crucial role in anchoring the Pt atom for its catalytic function. [1] B. Qiao, *etal.* Nat. Chem. 3 (2011) 634; B. Avasarala and P. Haldar, Int. J. Hydrog. Energy 36 (2011) 3965

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Date submitted: 09 Nov 2011

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