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**A DFT study of oxygen reduction reaction on single-atom Pt nanocatalyst** YOUNGJOO TAK, NORINA A. RICHTER, ALOYSIUS SOON, Global E3 Institute, Department of Materials Science and Engineering, YonseiUniversity, Seoul 120-749, Korea — Platinum is one of the most broadly used catalyst for many chemical reactions (e.g. oxygen reduction reaction). Although its great reactivity, platinum catalysis has not met enthusiastic reception from industry due to its high price. Pt/C catalyst is widely used to come over this problem, but still considered as an imperfect solution because of its poor stability [1,2]. Recently, platinum single-atom catalyst with TiN support has suggested and proved to be stable on the N vacancy site of TiN support under N-lean condition [3]. In this work, we present density-functional theory (DFT) study of the oxygen reduction reaction on single Pt atom embedded on the surfaces of TiN(100) and TiC(100) within the computational hydrogen model (CHE) [4].

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Youngjoo Tak
Global E3 Institute, Department of Materials Science and Engineering,
YonseiUniversity, Seoul 120-749, Korea

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