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Density Functional Theory Study of Oxygen Reduction Reaction Mechanism on $Pt_3Ti(111)$ Surface SHYAM KATTEL, Department of Mechanical Engineering and Materials Science, University of Pittsburgh, ZHIYAO DUAN, GUOFENG WANG, University of Pittsburgh — Density functional theory (DFT) calculations are performed to explain the ORR mechanism on Pt segregated $Pt_3Ti(111)$ surface. The possible ORR mechanism is elucidated by calculating the activation energies of all ORR elementary reaction steps. Our preliminary results predict that the ORR proceeds via a H_2O_2 dissociation mechanism with coverage dependent kinetics. At high coverage, the rate determining step (RDS) is protonation of adsorbed O_2 to form OOH. The energy barrier for this process is 0.20 eV which is lower than the energy barrier for RDS on pure Pt(111) surface. These findings suggest that modified PtTi(111) surface has better ORR activity in comparison to pure Pt(111) surface. Furthermore, we have studied the corrosion behavior of $Pt_3Ti(111)$ surface by evaluating the electrochemical potential shift for clean and oxygenated surface. The computations predict enhanced stability of $Pt_3Ti(111)$ surface against surface Pt dissolution in comparison to Pt dissolution from pure Pt(111) surface.

Shyam Kattel
Dept of Mechanical Engineering and Materials Science,
University of Pittsburgh

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