# PHYSICS COLLOQUIUM

## Combined First-Principles Molecular Dynamics / Density-Functional Theory Study of Ammonia Oxidation on Pt(100) Electrode

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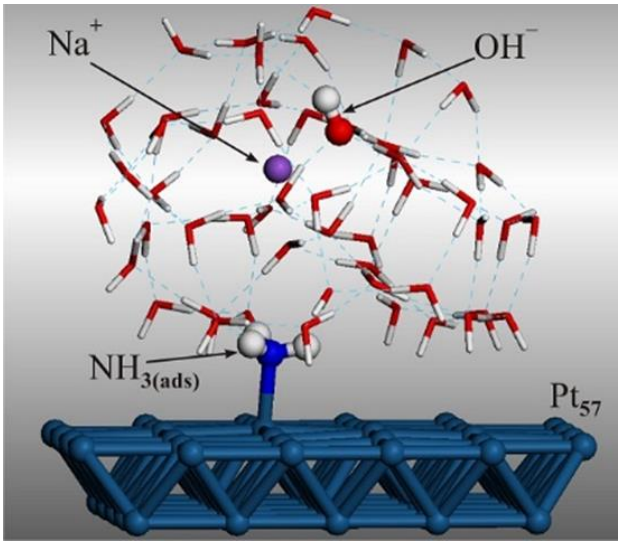
A combined first-principles molecular dynamics / density functional theory study of the electrooxidation of ammonia is conducted to gain an atomic-level understanding of the electrocatalytic processes at the Pt(100) / alkaline solution interface and to probe the mechanistic details of ammonia electrooxidation on the metal surface. A systematic study of adsorption and relative stability of ammonia and the intermediate species on the Pt(100) surface as a function of potential is carried out and activation energy profiles for the mechanistic steps in the ammonia oxidation are presented. The reaction mechanism is potential dependent: the modeling study supports the Oswin and Salomon's mechanism for moderate surface potentials (≥ +0.5 V vs. RHE), and the Gerischer and Maurer's mechanism for lower potentials (< +0.5 V vs. RHE). The high electrocatalytic activity of Pt(100) is ascribed to the facile dimerization of bridging nitrogen atoms to form molecular nitrogen, whereas low activity of Pt(111) and Pt(110) is imputed to the nitrogen atoms that are strongly bound at hollow sites and poisoning the surface.




**April 14, 2021**
**4:00 pm**
**Zoom Meeting**

*Everyone Welcome!*