Oxygen reduction reaction (ORR) is one of the most important rate-limiting steps in the catalytical water formation reaction in hydrogen based low temperature fuel cells. Platinum has been widely used as industrialized catalyst to enable the use of fuel cell. Recent results show that platinum-base alloy can serve as a better candidate for catalyst of next generation.

To understand the reaction details in ORR reaction, we theoretically studied the catalytical ORR on eleven transition metals. Adsorption property, reaction intermediates and the corresponding barriers involved in the water formation are studied. OH formation, OOH formation and water formation are observed to be the rate determined step for the ORR on different metals. Pd and Cu showed similar potential energy surface to Pt and are hence best candidate for the development of less expensive catalysts.