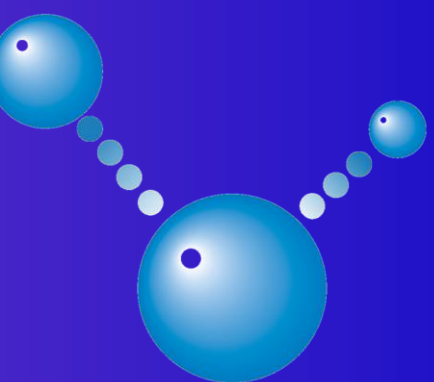


Computational Quantum Chemistry Analysis of the Cathodic Catalyst in Low Temperature Fuel Cells

低溫燃料電池陰極觸媒量子化學計算分析

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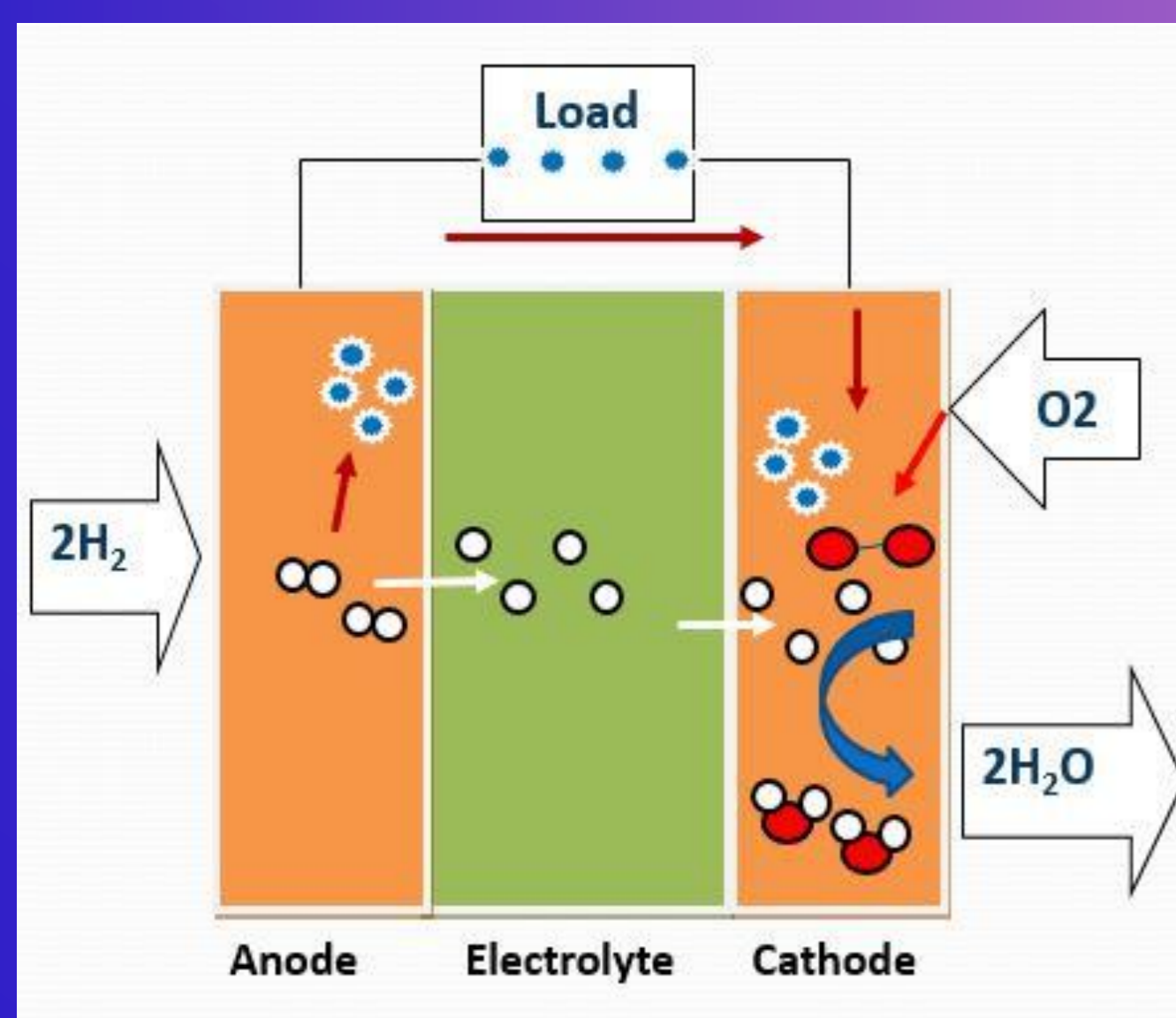


Green Energy & Molecular Engineering Lab

Objective

- To improve the efficiency of fuel cells by Pt doped carbon based supporters.
- To simulate the oxygen reduction reaction (ORR) at the cathodic catalysts by employing computational quantum chemistry techniques (Density Functional Theory, DFT).
- To predict the catalytic activities of the ORR via various catalysts and supporters.

Fuel cell Mechanics



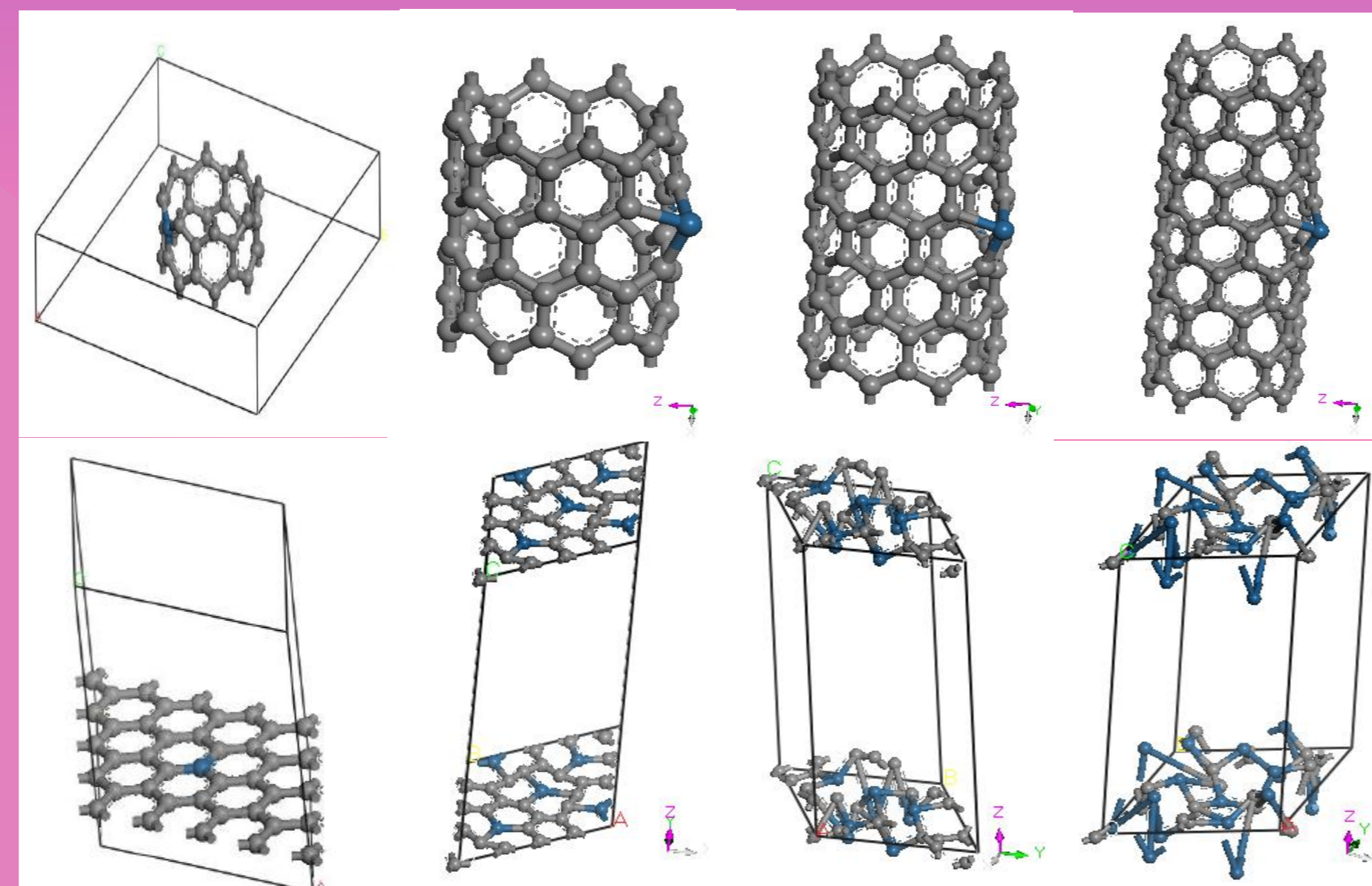
Kohn-Sham Equation

$$\left(-\frac{\hbar^2}{2m} \nabla^2 + V_{effect} \right) \psi_i(\mathbf{r}) = \varepsilon_i \psi_i(\mathbf{r})$$

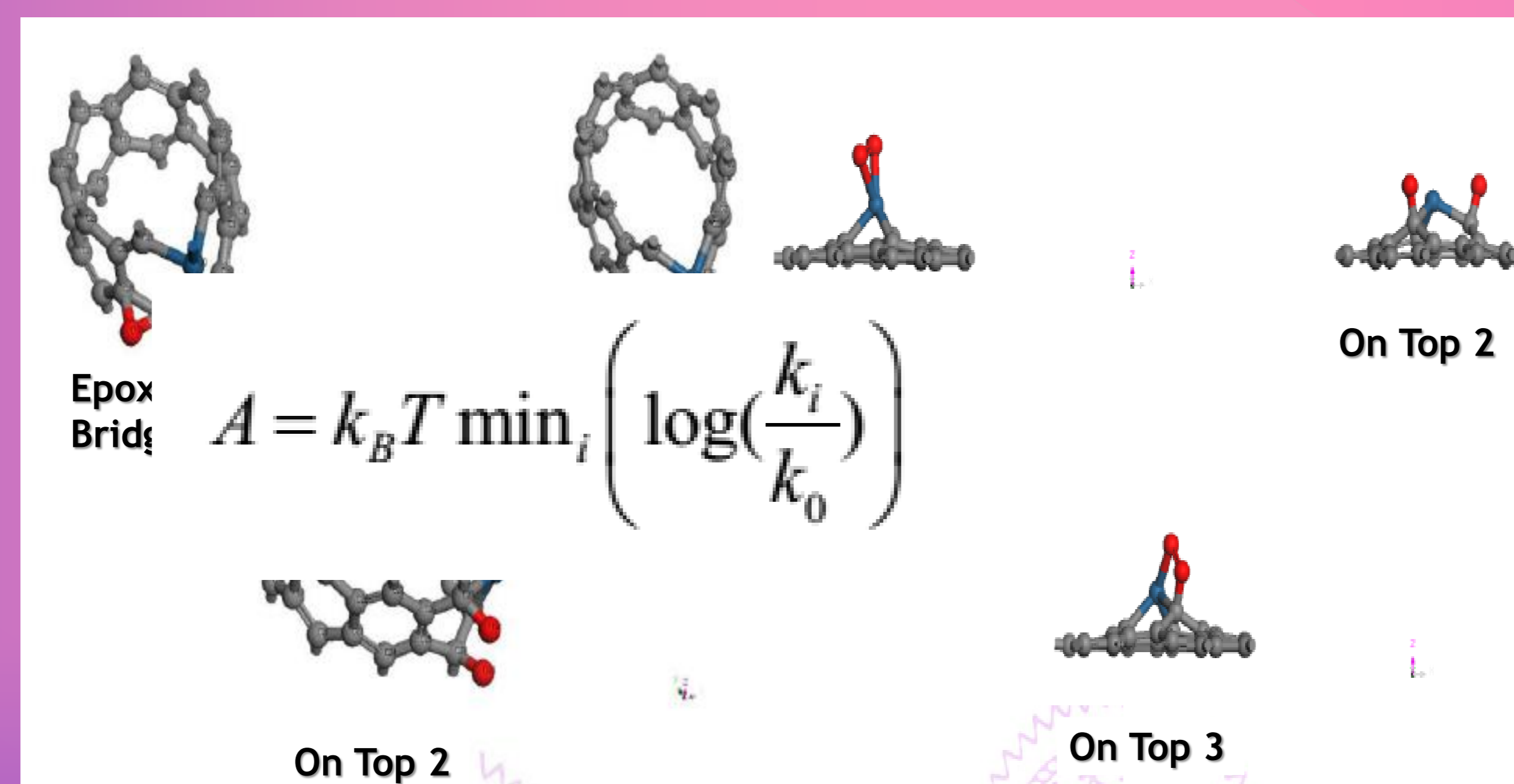
Sabatier Analysis

$$A = k_B T \min_i \left(\log \left(\frac{k_i}{k_0} \right) \right)$$

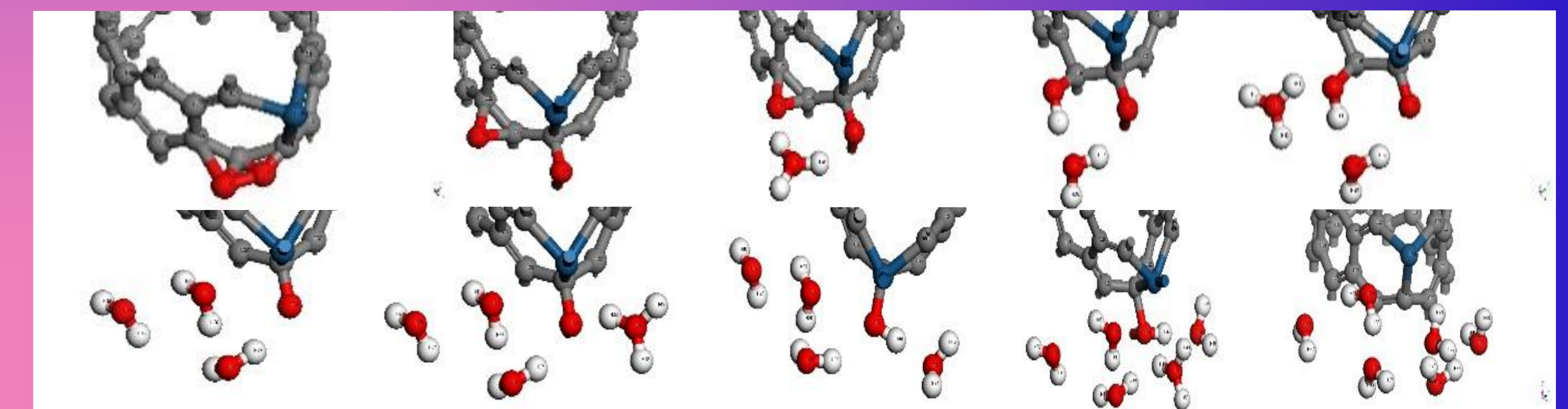
Molecular Structure



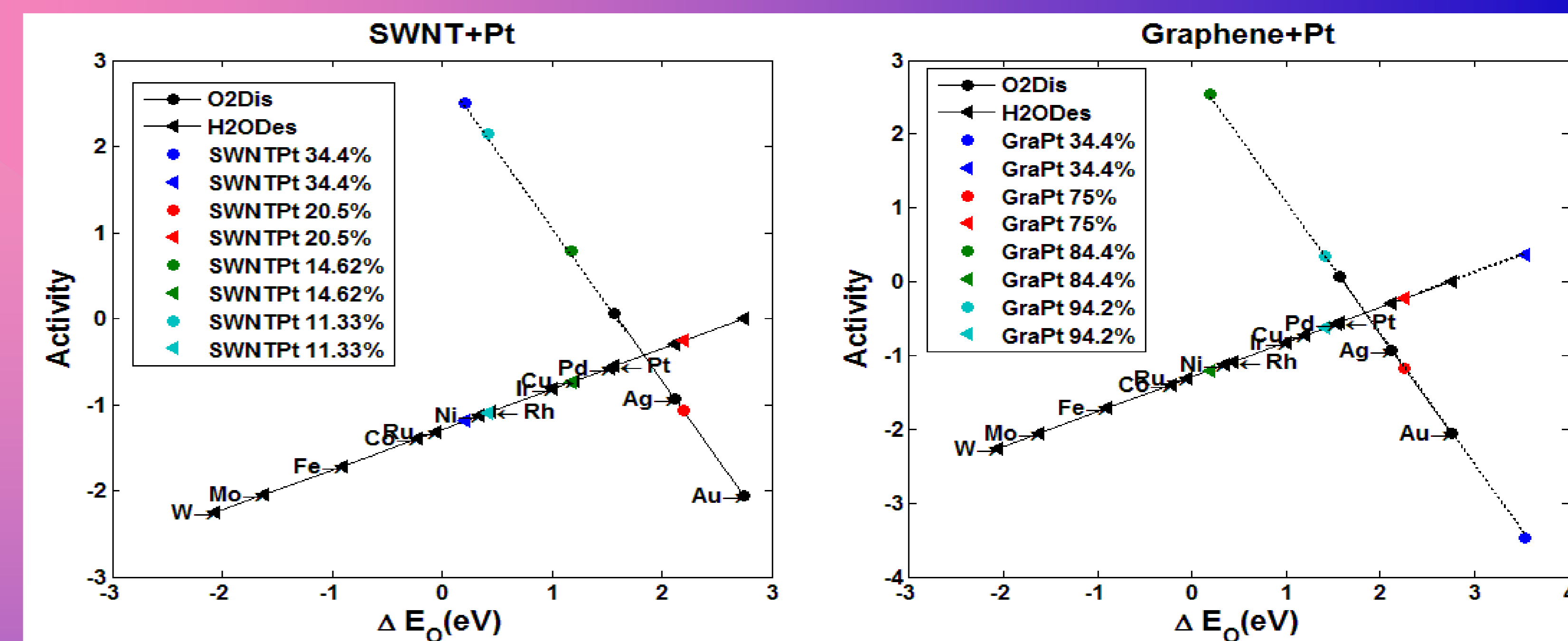
Adsorption Type



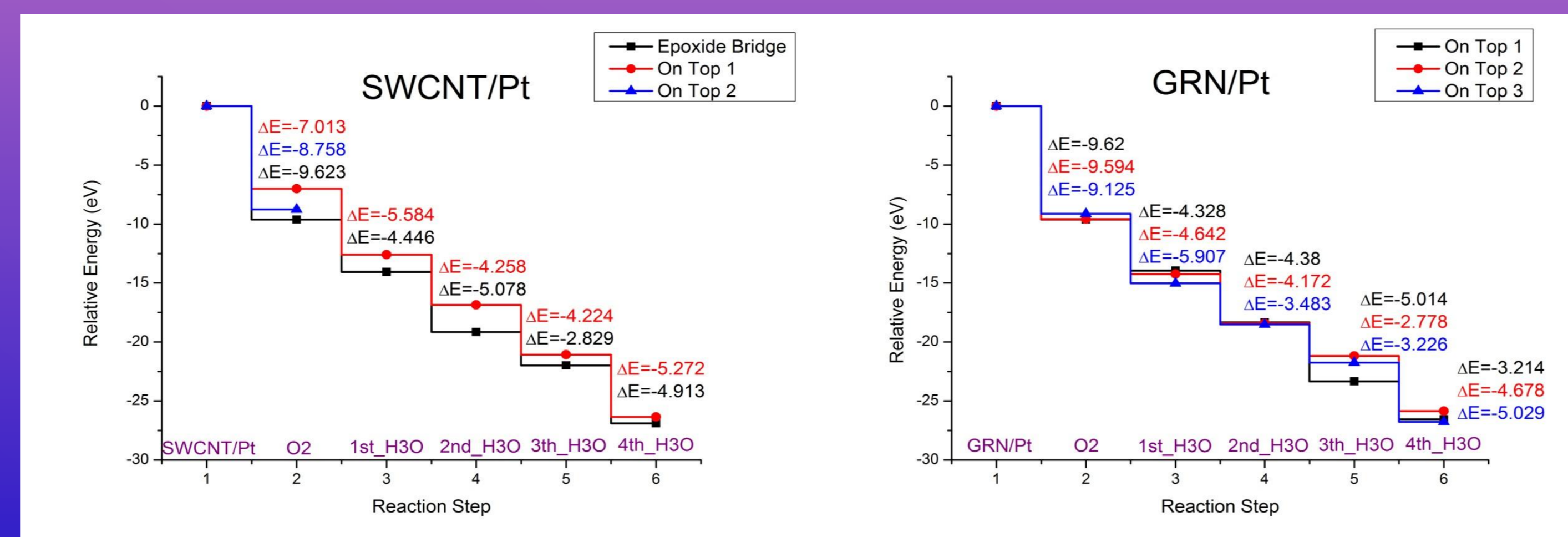
Major Steps of the ORR at the Cathode



Catalyst activity & volcano curve



Analysis of Relative energy in each ORR steps



Catalyst activity V.S. Pt wt%

