

Article

Adsorption Energy Shifts for Oxygen and Hydroxyl on 4-atom Metal-Decorated Graphene Catalysts Via Solvation, pH, and Substrate Dopants: Effects on ORR Activity

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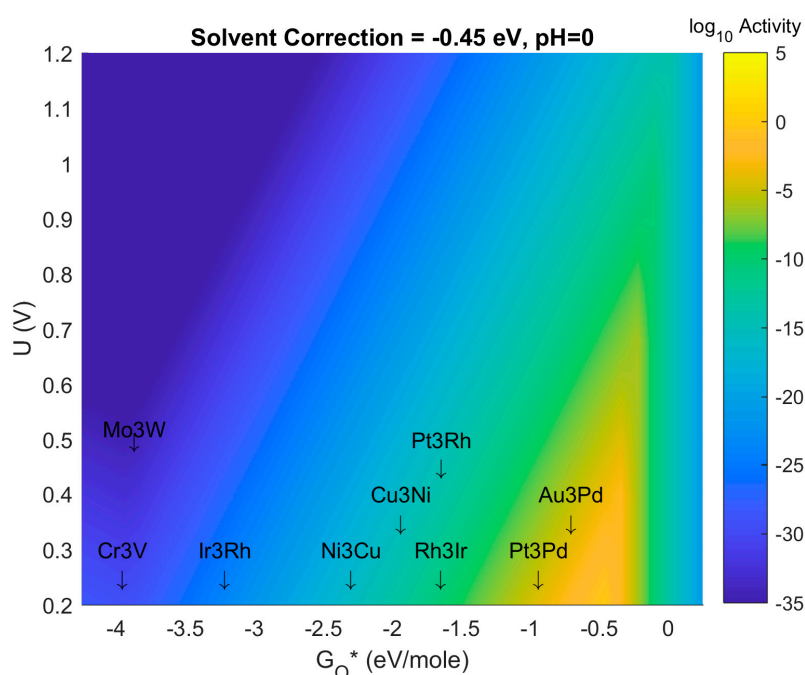


Figure SI 1a. Zoomed in From Figure 6 of Main Document Volcano Plot analysis for ORR activity at solvent correction value of -0.45 eV. **Top left** (pH = 0), Top right (pH = 1), Bottom left (pH = 3), Bottom right (pH = 7). Blue denotes lowest activity, yellow denotes highest activity. All plots use same color-axis scale hence some saturation at maximum activity and minimum activity. Activity given in log10 scale to show more detail in plot.

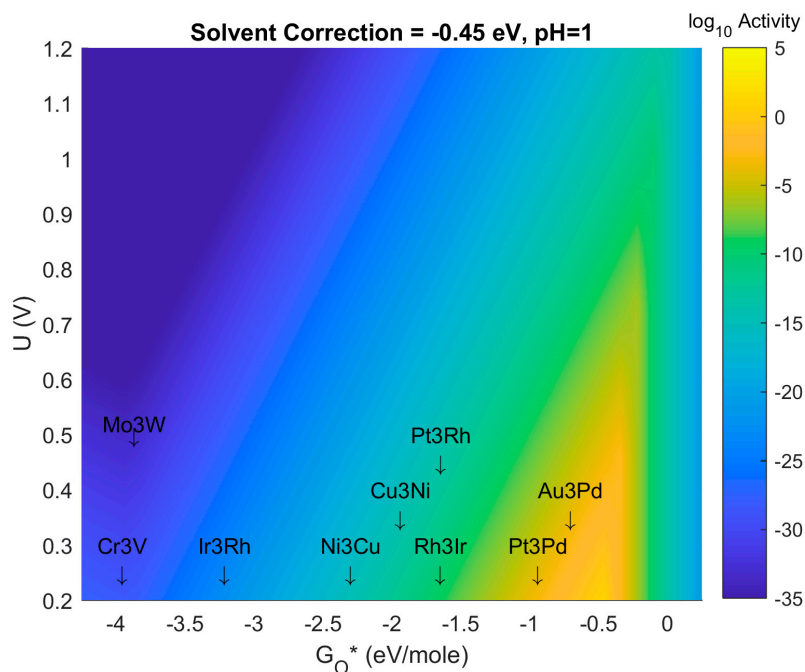


Figure SI 1b. Zoomed in From Figure 6 of Main Document Volcano Plot analysis for ORR activity at solvent correction value of -0.45 eV. Top left (pH = 0), **Top right** (pH = 1), Bottom left (pH = 3), Bottom right (pH = 7). Blue denotes lowest activity, yellow denotes highest activity. All plots use same color-axis scale hence some saturation at maximum activity and minimum activity. Activity given in log10 scale to show more detail in plot.

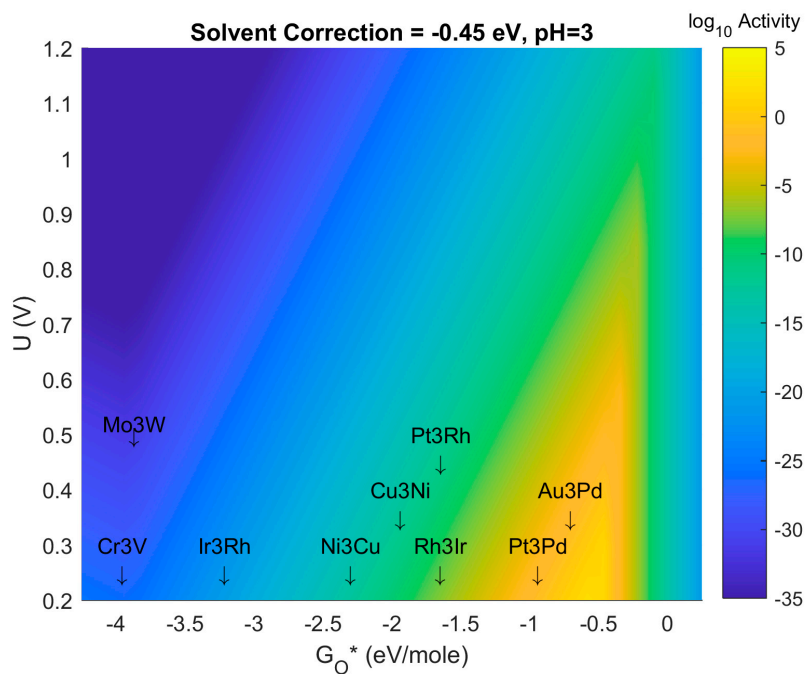


Figure SI 1c. Zoomed in From Figure 6 of Main Document Volcano Plot analysis for ORR activity at solvent correction value of -0.45 eV. Top left (pH = 0), Top right (pH = 1), **Bottom left** (pH = 3), Bottom right (pH = 7). Blue denotes lowest activity, yellow denotes highest activity. All plots use same color-axis scale hence some saturation at maximum activity and minimum activity. Activity given in log10 scale to show more detail in plot.

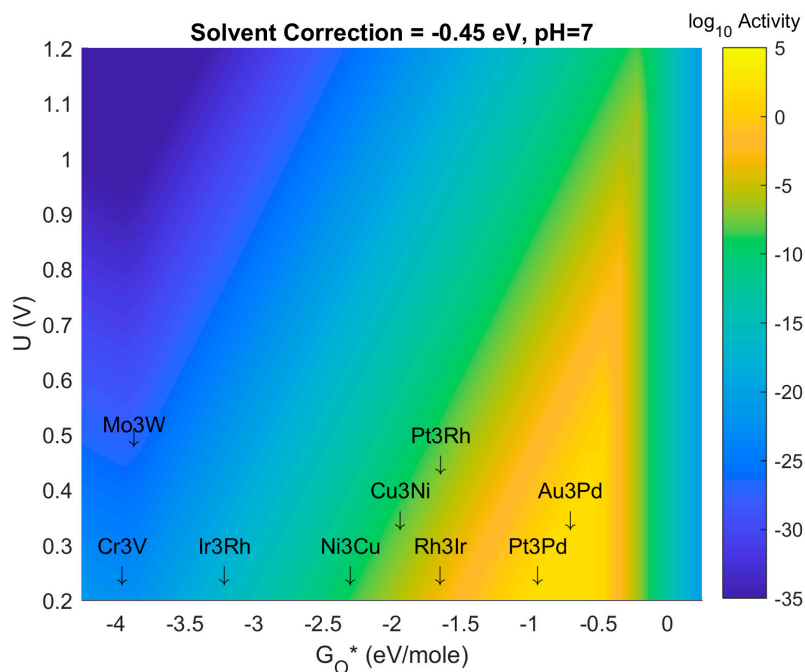


Figure SI 1d. Zoomed in From Figure 6 of Main Document Volcano Plot analysis for ORR activity at solvent correction value of -0.45 eV. Top left (pH = 0), Top right (pH = 1), Bottom left (pH = 3), **Bottom right** (pH = 7). Blue denotes lowest activity, yellow denotes highest activity. All plots use same color-axis scale hence some saturation at maximum activity and minimum activity. Activity given in log10 scale to show more detail in plot.

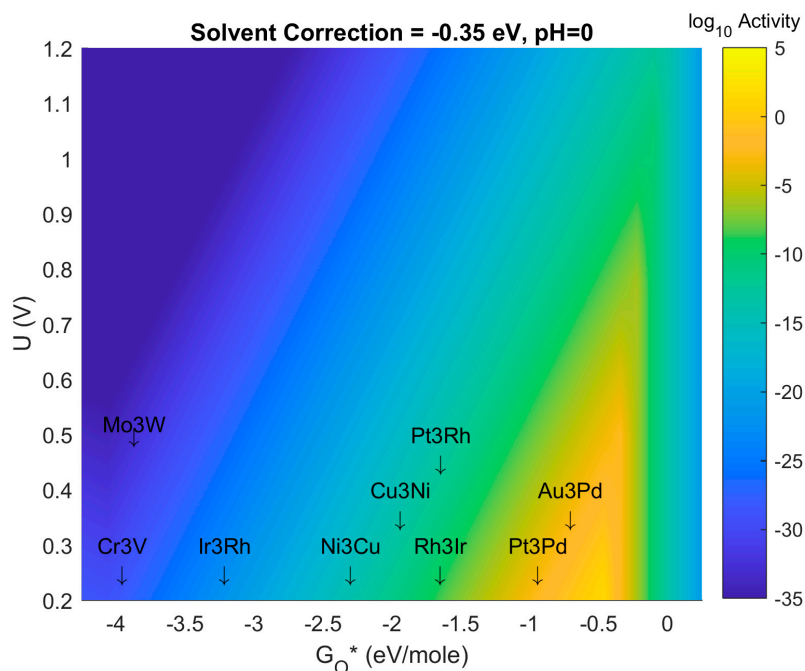


Figure SI 2a. Zoomed in From Figure 7 of Main Document Volcano Plot analysis for ORR activity at solvent correction value of -0.35 eV. **Top left** (pH = 0), Top right (pH = 1), Bottom left (pH = 3), Bottom right (pH = 7). Blue denotes lowest activity, yellow denotes highest activity. All plots use same color-axis scale hence some saturation at maximum activity and minimum activity. Activity given in log10 scale to show more detail in plot.

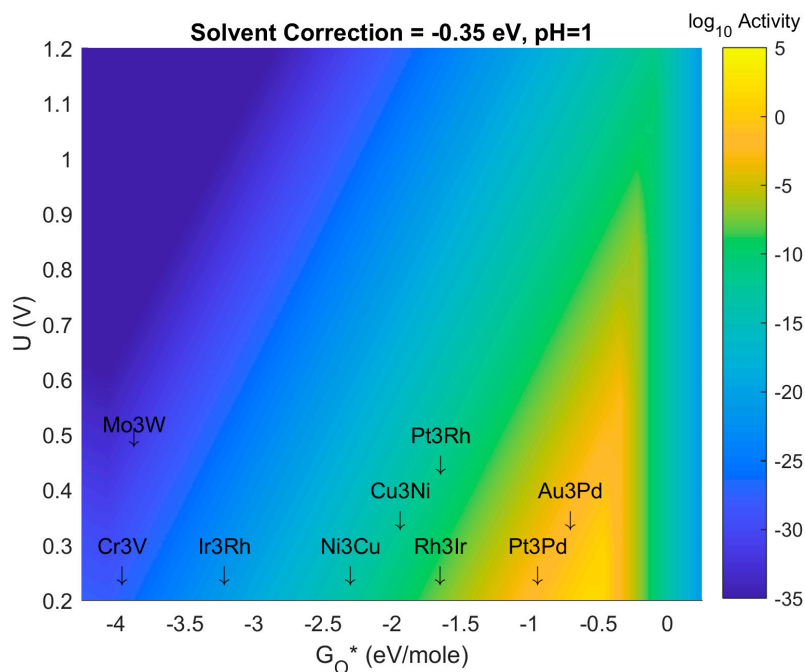


Figure SI 2b. Zoomed in From Figure 7 of Main Document Volcano Plot analysis for ORR activity at solvent correction value of -0.35 eV. Top left (pH = 0), **Top right** (pH = 1), Bottom left (pH = 3), Bottom right (pH = 7). Blue denotes lowest activity, yellow denotes highest activity. All plots use same color-axis scale hence some saturation at maximum activity and minimum activity. Activity given in log10 scale to show more detail in plot.

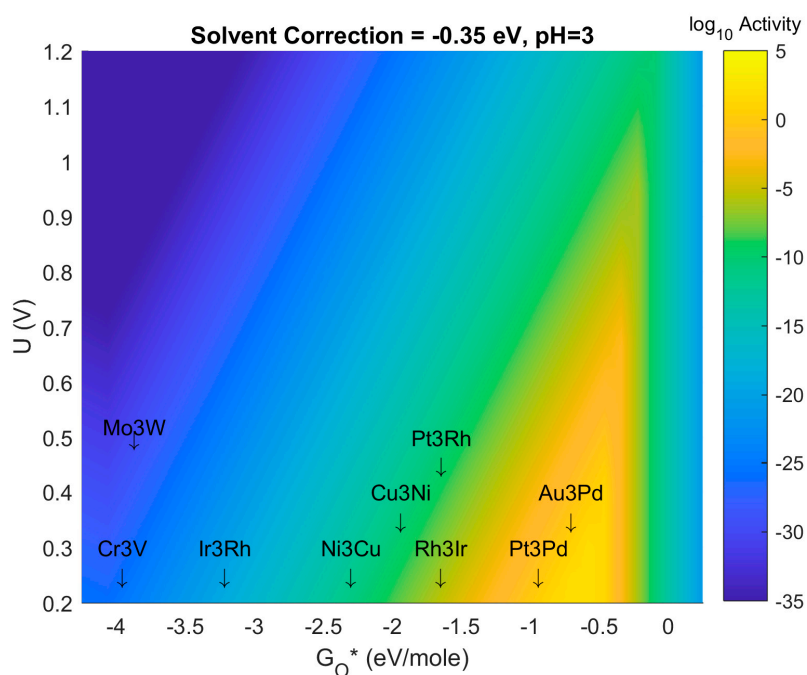


Figure SI 2c. Zoomed in From Figure 7 of Main Document Volcano Plot analysis for ORR activity at solvent correction value of -0.35 eV. Top left (pH = 0), Top right (pH = 1), **Bottom left** (pH = 3), Bottom right (pH = 7). Blue denotes lowest activity, yellow denotes highest activity. All plots use same color-axis scale hence some saturation at maximum activity and minimum activity. Activity given in log10 scale to show more detail in plot.

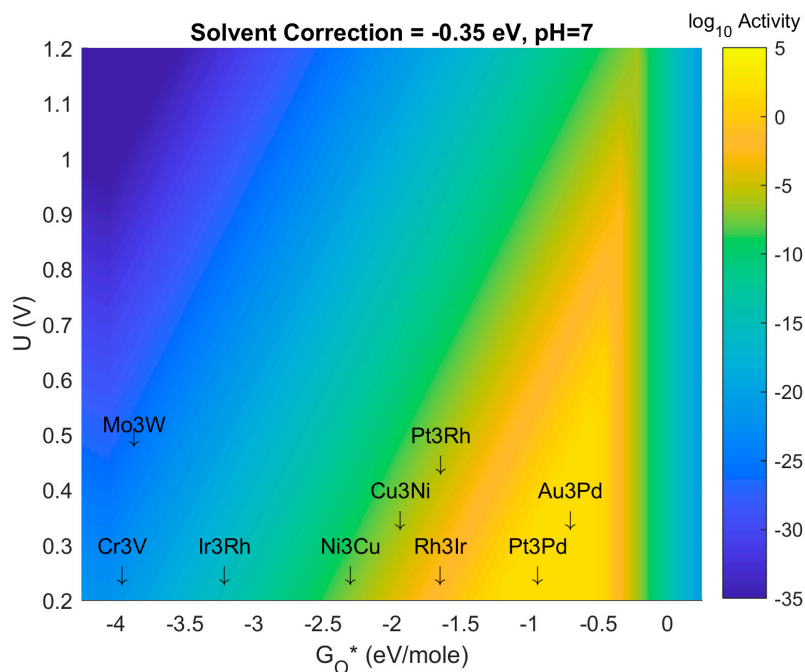


Figure SI 2d. Zoomed in From Figure 7 of Main Document Volcano Plot analysis for ORR activity at solvent correction value of -0.35 eV. Top left (pH = 0), Top right (pH = 1), Bottom left (pH = 3), **Bottom right** (pH = 7). Blue denotes lowest activity, yellow denotes highest activity. All plots use same color-axis scale hence some saturation at maximum activity and minimum activity. Activity given in \log_{10} scale to show more detail in plot.

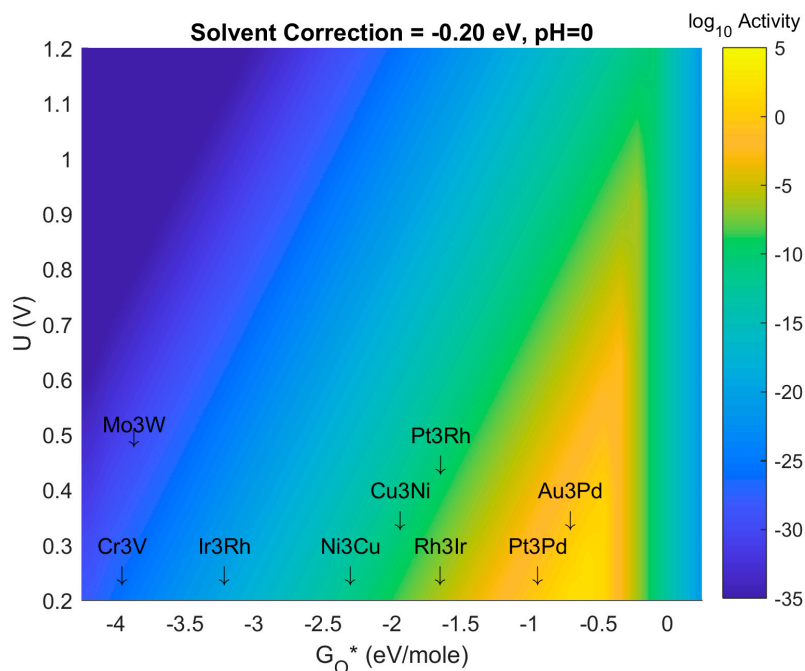


Figure SI 3a. Zoomed in From Figure 8 of Main Document Volcano Plot analysis for ORR activity at solvent correction value of -0.20 eV. **Top left** (pH = 0), Top right (pH = 1), Bottom left (pH = 3), Bottom right (pH = 7). Blue denotes lowest activity, yellow denotes highest activity. All plots use same color-axis scale hence some saturation at maximum activity and minimum activity. Activity given in \log_{10} scale to show more detail in plot.

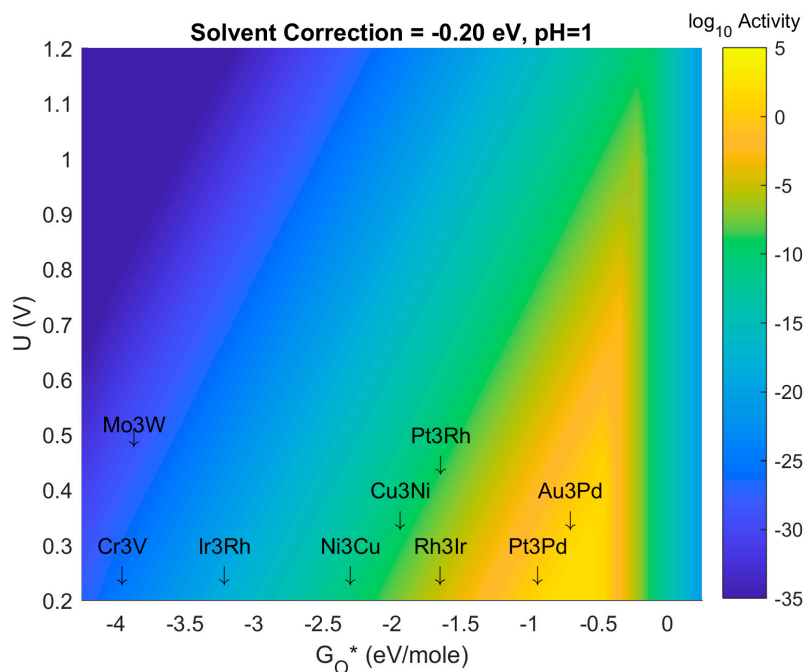


Figure SI 3b. Zoomed in From Figure 8 of Main Document Volcano Plot analysis for ORR activity at solvent correction value of -0.20 eV. Top left (pH = 0), **Top right** (pH = 1), Bottom left (pH = 3), Bottom right (pH = 7). Blue denotes lowest activity, yellow denotes highest activity. All plots use same color-axis scale hence some saturation at maximum activity and minimum activity. Activity given in log10 scale to show more detail in plot.

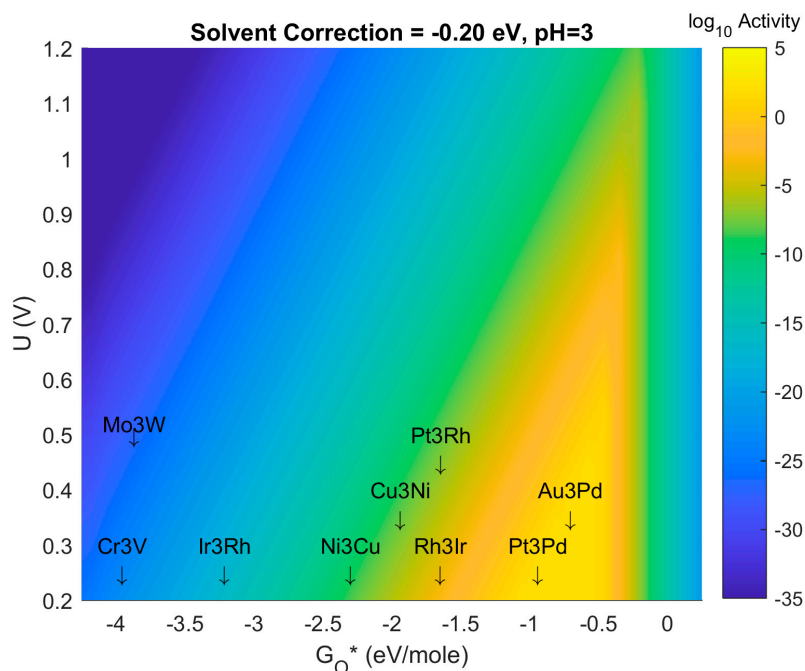


Figure SI 3c. Zoomed in From Figure 8 of Main Document Volcano Plot analysis for ORR activity at solvent correction value of -0.20 eV. Top left (pH = 0), Top right (pH = 1), **Bottom left** (pH = 3), Bottom right (pH = 7). Blue denotes lowest activity, yellow denotes highest activity. All plots use same color-axis scale hence some saturation at maximum activity and minimum activity. Activity given in log10 scale to show more detail in plot.

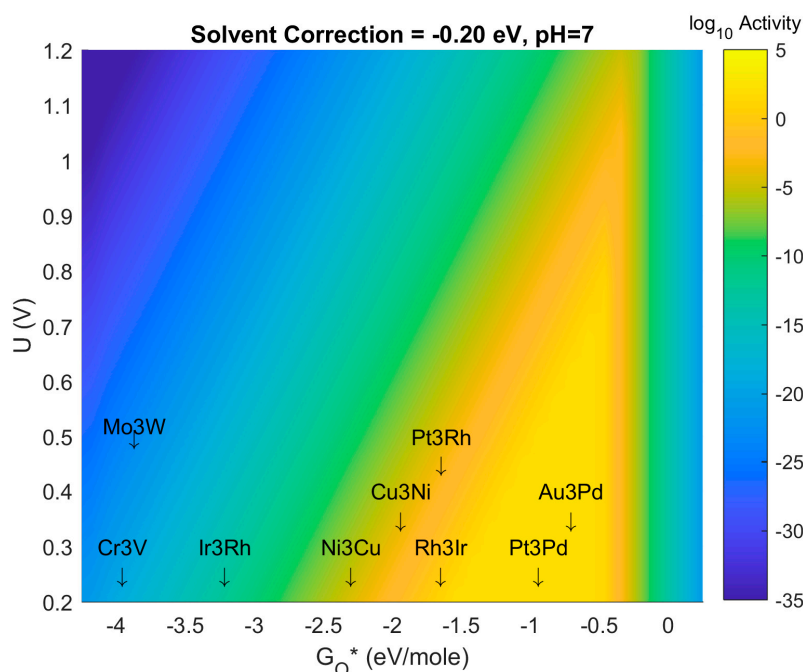


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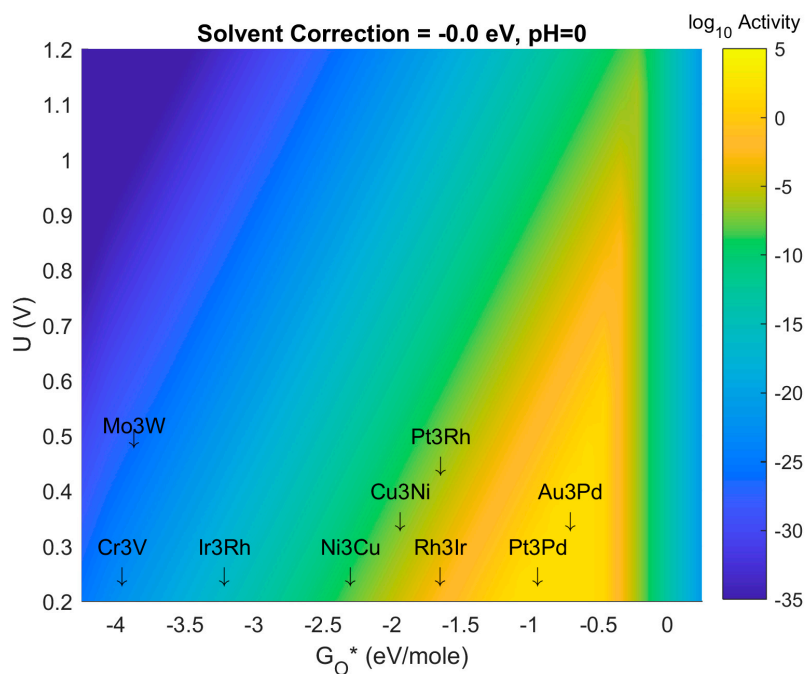


Figure SI 4a. Zoomed in From Figure 9 of Main Document Volcano Plot analysis for ORR activity at solvent correction value of -0.00 eV. **Top left** (pH = 0), Top right (pH = 1), Bottom left (pH = 3), Bottom right (pH = 7). Blue denotes lowest activity, yellow denotes highest activity. All plots use same color-axis scale hence some saturation at maximum activity and minimum activity. Activity given in \log_{10} scale to show more detail in plot.

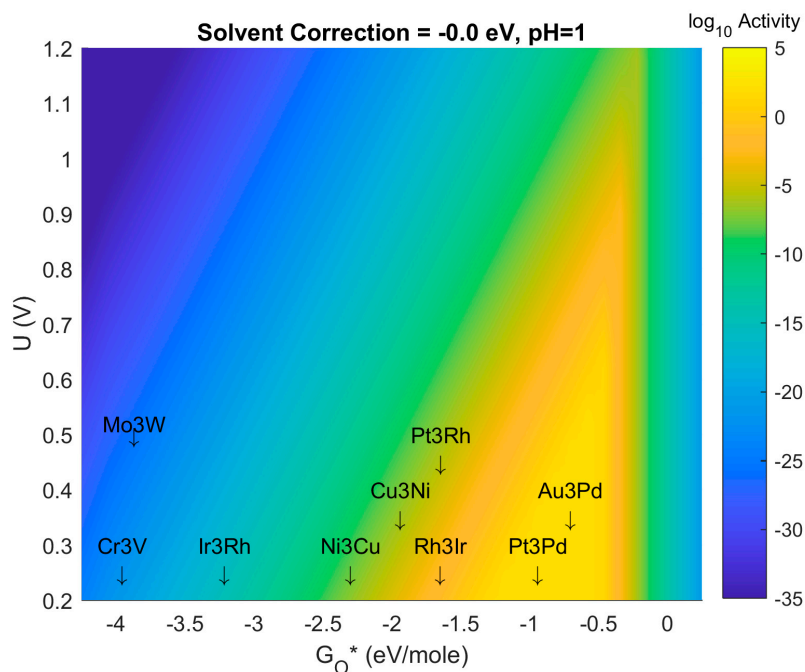


Figure SI 4b. Zoomed in From Figure 9 of Main Document Volcano Plot analysis for ORR activity at solvent correction value of -0.00 eV. Top left (pH = 0), **Top right** (pH = 1), Bottom left (pH = 3), Bottom right (pH = 7). Blue denotes lowest activity, yellow denotes highest activity. All plots use same color-axis scale hence some saturation at maximum activity and minimum activity. Activity given in log₁₀ scale to show more detail in plot.

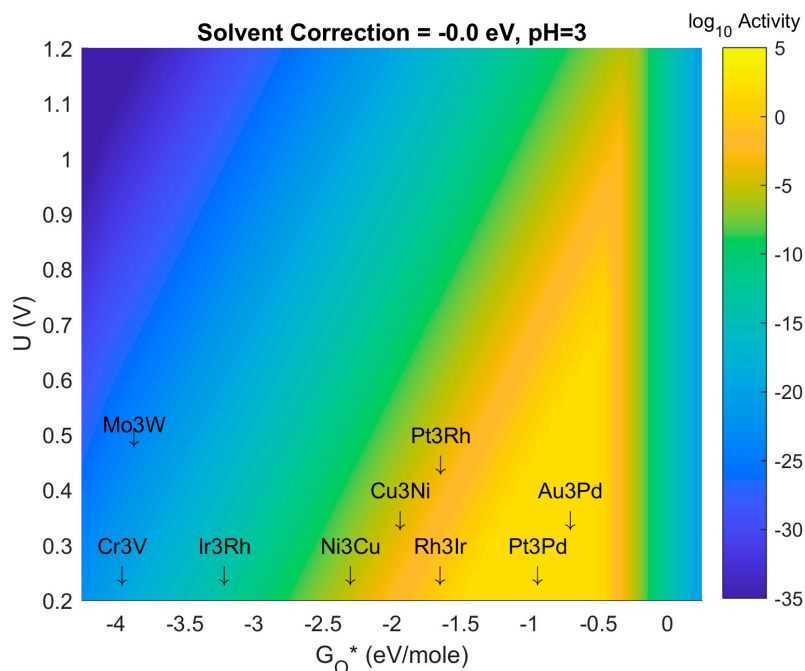


Figure SI 4c. Zoomed in From Figure 9 of Main Document Volcano Plot analysis for ORR activity at solvent correction value of -0.00 eV. Top left (pH = 0), Top right (pH = 1), **Bottom left** (pH = 3), Bottom right (pH = 7). Blue denotes lowest activity, yellow denotes highest activity. All plots use same color-axis scale hence some saturation at maximum activity and minimum activity. Activity given in log₁₀ scale to show more detail in plot.

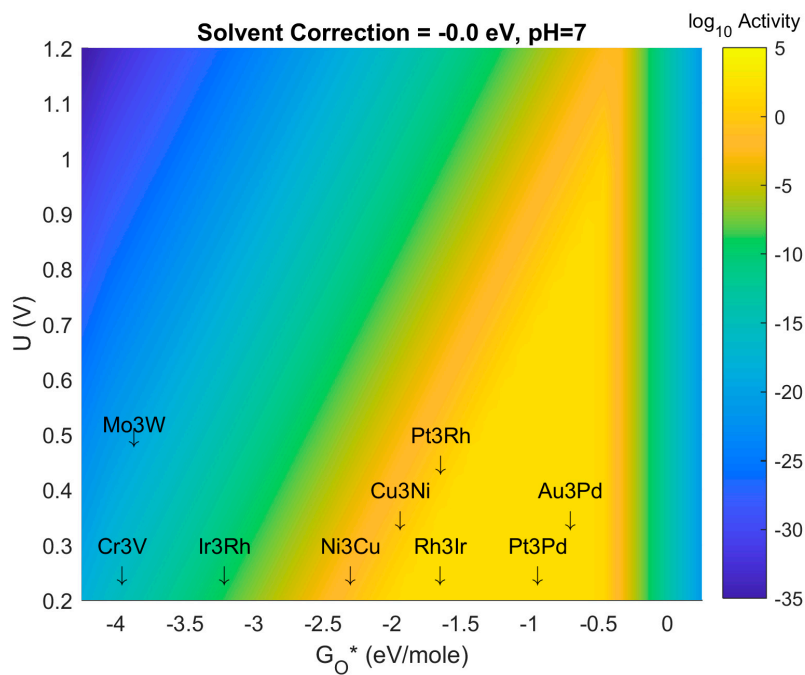


Figure SI 4d. Zoomed in From Figure 9 of Main Document Volcano Plot analysis for ORR activity at solvent correction value of -0.00 eV. Top left (pH = 0), Top right (pH = 1), Bottom left (pH = 3), **Bottom right** (pH = 7). Blue denotes lowest activity, yellow denotes highest activity. All plots use same color-axis scale hence some saturation at maximum activity and minimum activity. Activity given in \log_{10} scale to show more detail in plot.