

Article

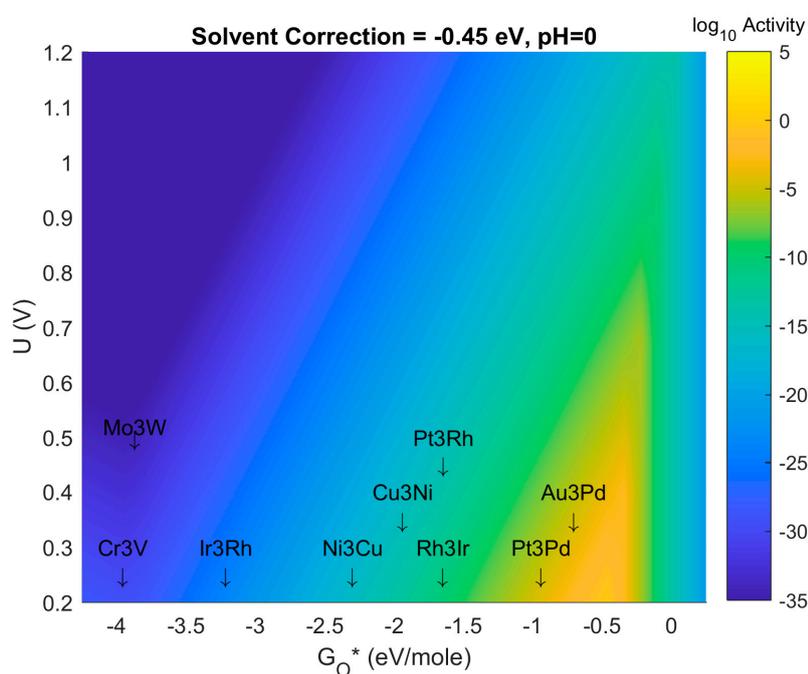
# Adsorption Energy Shifts for Oxygen and Hydroxyl on 4-atom Metal-Decorated Graphene Catalysts Via Solvation, pH, and Substrate Dopants: Effects on ORR Activity

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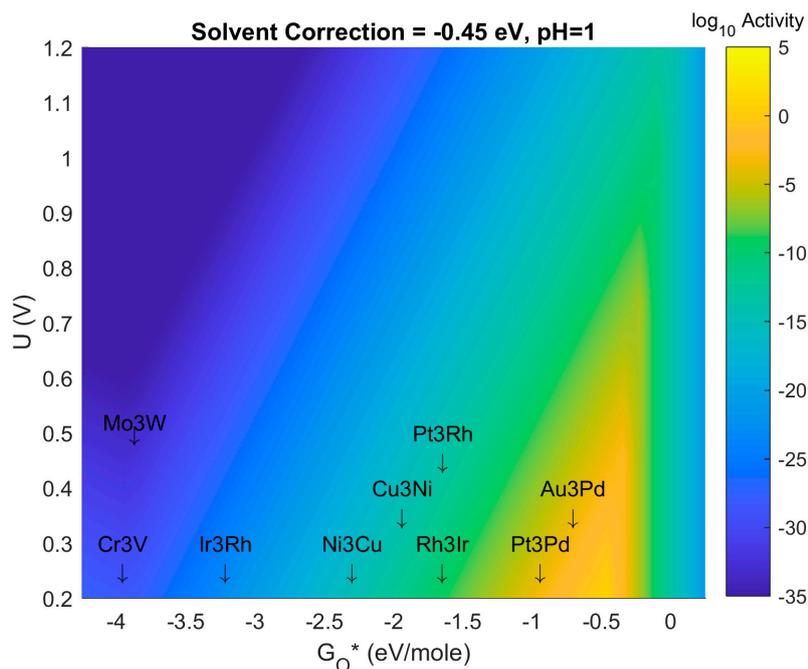
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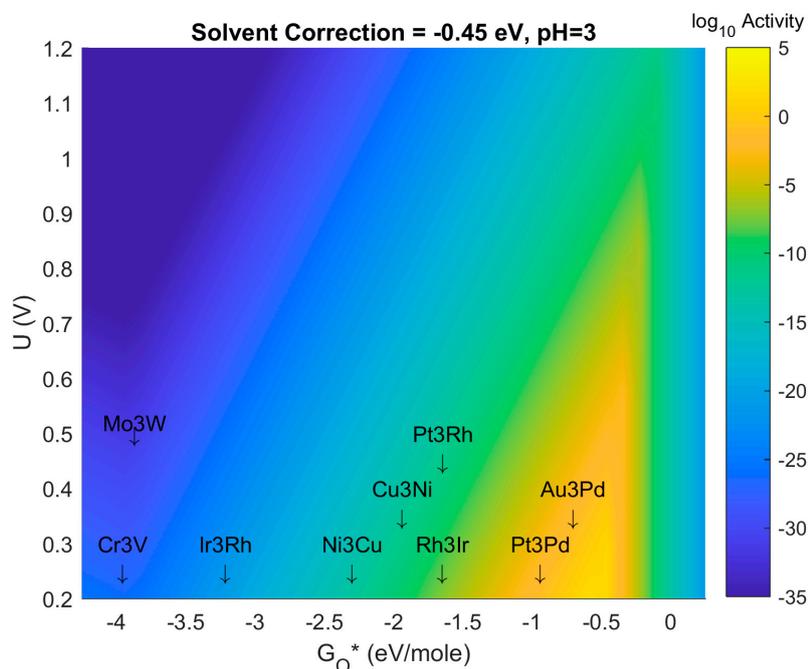
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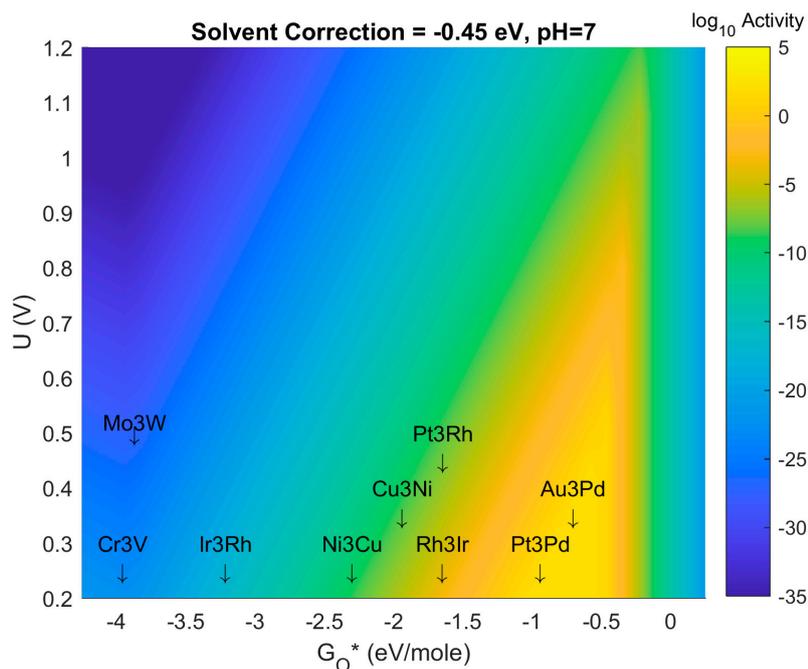
**Figure SI 1a.** Zoomed in From Figure 6 of Main Document Volcano Plot analysis for ORR activity at solvent correction value of -0.45 eV. **Top left** (pH = 0), **Top right** (pH = 1), **Bottom left** (pH = 3), **Bottom right** (pH = 7). Blue denotes lowest activity, yellow denotes highest activity. 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.



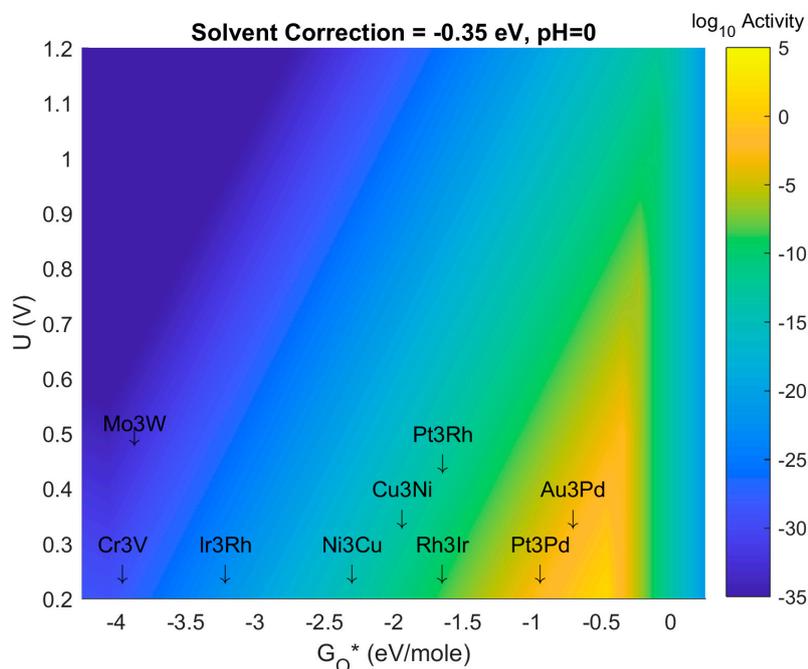
**Figure SI 1b.** Zoomed in From Figure 6 of Main Document Volcano Plot analysis for ORR activity at solvent correction value of  $-0.45$  eV. Top left (pH = 0), **Top right** (pH = 1), Bottom left (pH = 3), Bottom right (pH = 7). Blue denotes lowest activity, yellow denotes highest activity. All plots use same color-axis scale hence some saturation at maximum activity and minimum activity. Activity given in  $\log_{10}$  scale to show more detail in plot.



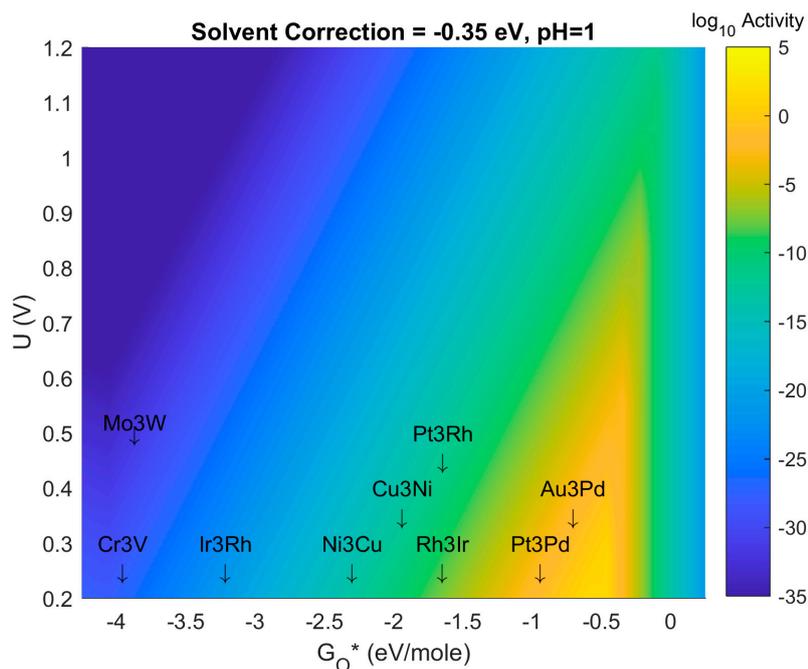
**Figure SI 1c.** Zoomed in From Figure 6 of Main Document Volcano Plot analysis for ORR activity at solvent correction value of  $-0.45$  eV. Top left (pH = 0), Top right (pH = 1), **Bottom left** (pH = 3), Bottom right (pH = 7). Blue denotes lowest activity, yellow denotes highest activity. All plots use same color-axis scale hence some saturation at maximum activity and minimum activity. Activity given in  $\log_{10}$  scale to show more detail in plot.



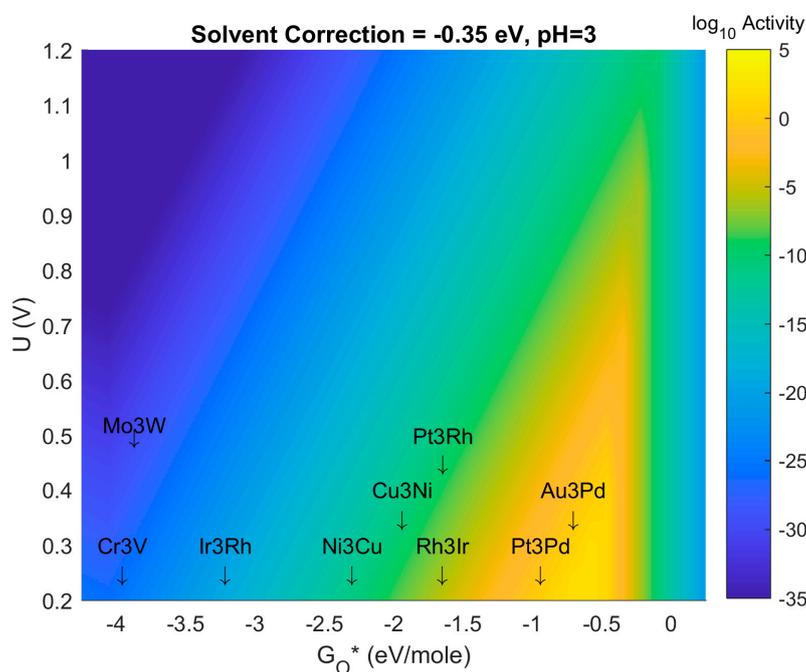
**Figure SI 1d.** Zoomed in From Figure 6 of Main Document Volcano Plot analysis for ORR activity at solvent correction value of  $-0.45$  eV. Top left (pH = 0), Top right (pH = 1), Bottom left (pH = 3), **Bottom right** (pH = 7). Blue denotes lowest activity, yellow denotes highest activity. All plots use same color-axis scale hence some saturation at maximum activity and minimum activity. Activity given in  $\log_{10}$  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  $\log_{10}$  scale to show more detail in plot.



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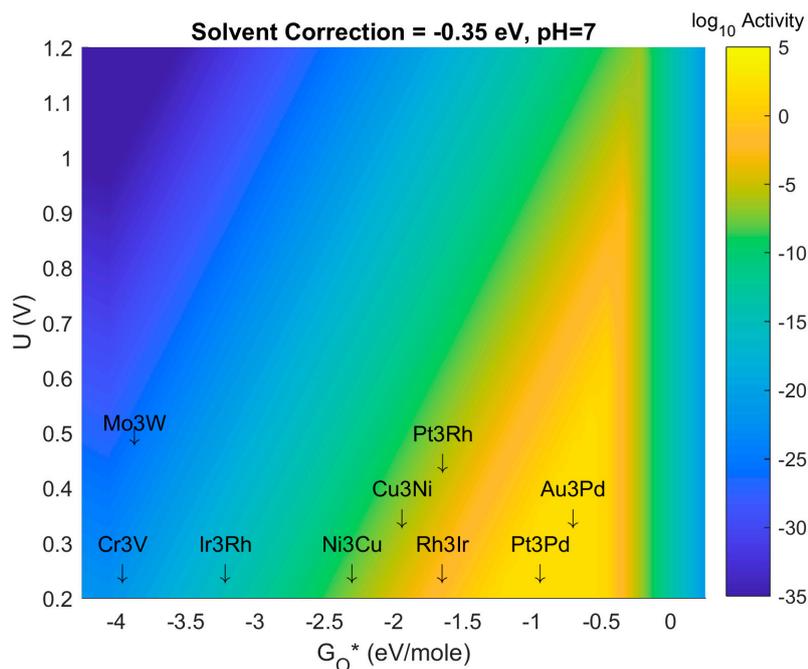
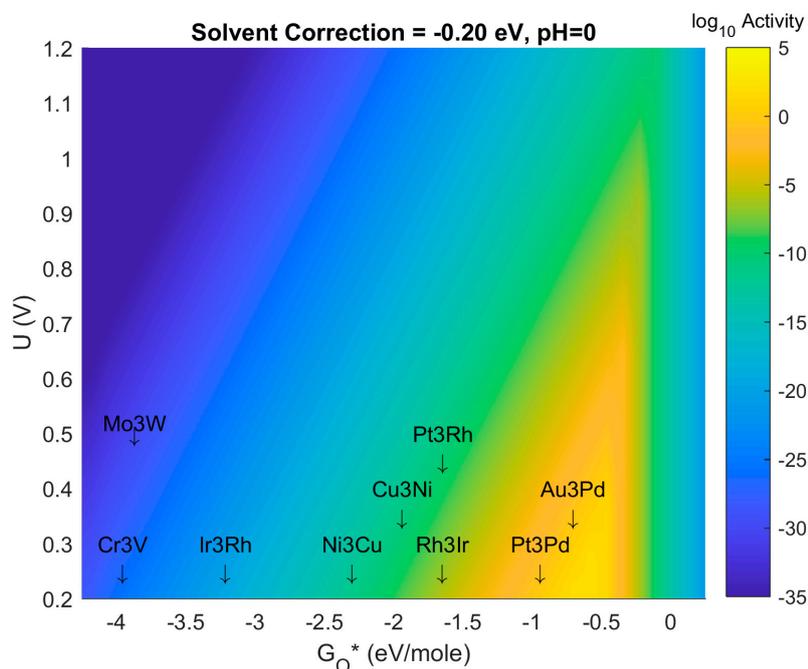
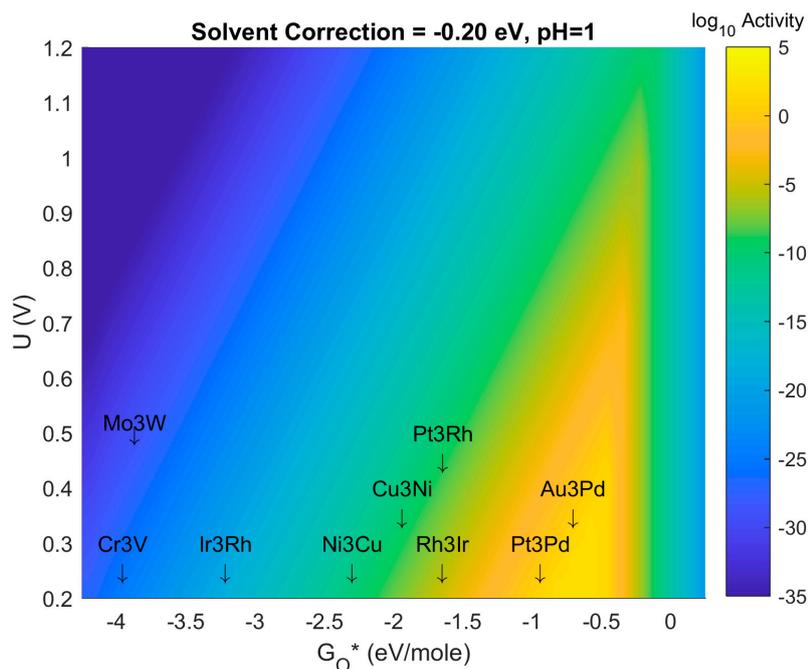


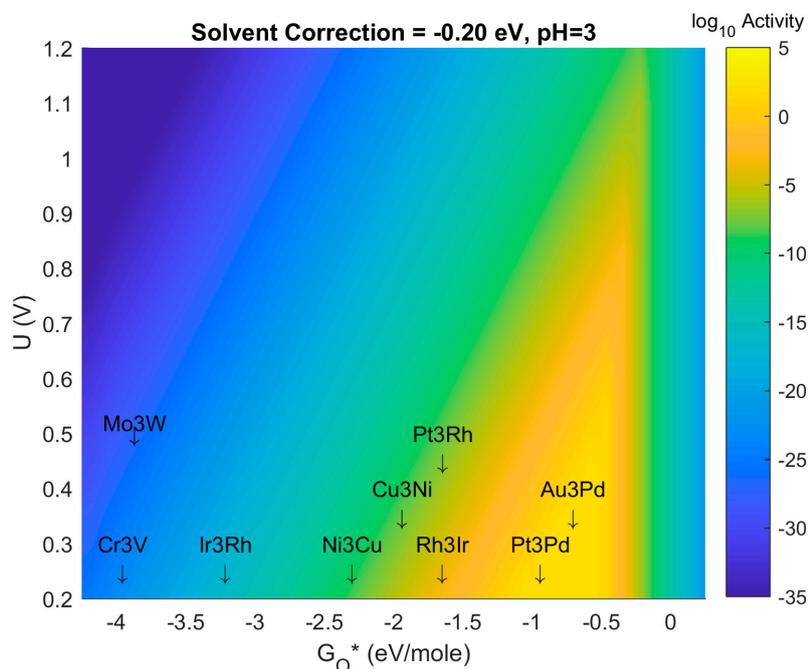
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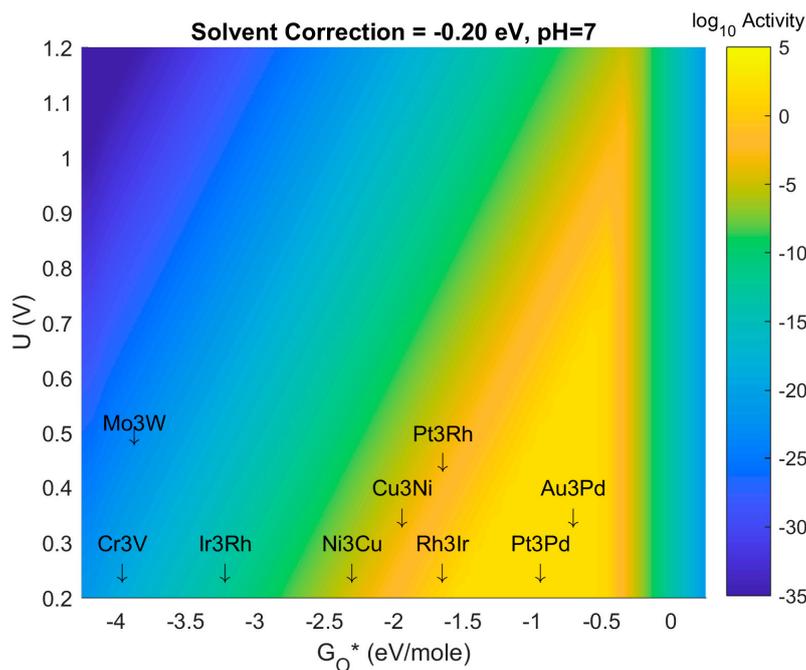
**Figure SI 3a.** Zoomed in From Figure 8 of Main Document Volcano Plot analysis for ORR activity at solvent correction value of  $-0.20$  eV. **Top left** (pH = 0), Top right (pH = 1), Bottom left (pH = 3), Bottom right (pH = 7). Blue denotes lowest activity, yellow denotes highest activity. All plots 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.



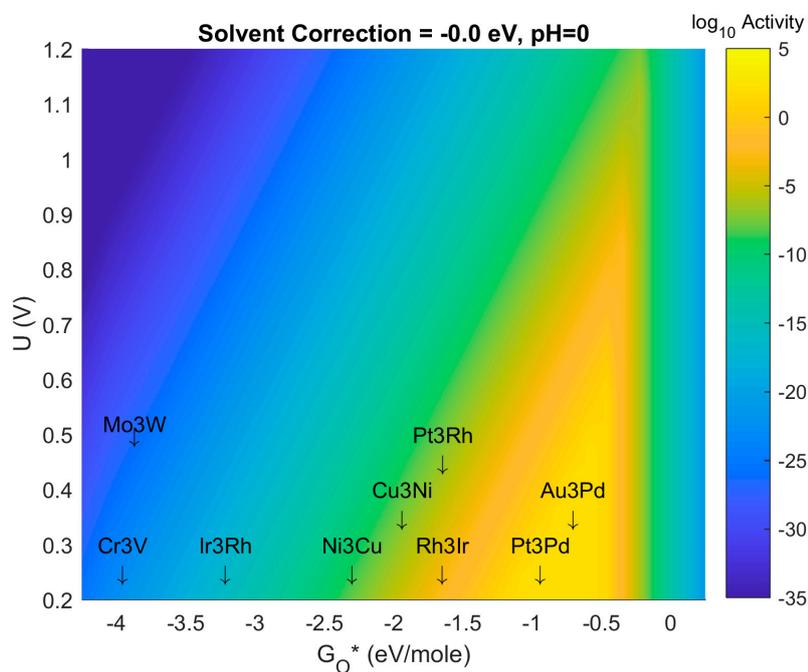
**Figure SI 3b.** Zoomed in From Figure 8 of Main Document Volcano Plot analysis for ORR activity at solvent correction value of  $-0.20$  eV. Top left (pH = 0), **Top right** (pH = 1), Bottom left (pH = 3), Bottom right (pH = 7). Blue denotes lowest activity, yellow denotes highest activity. All plots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



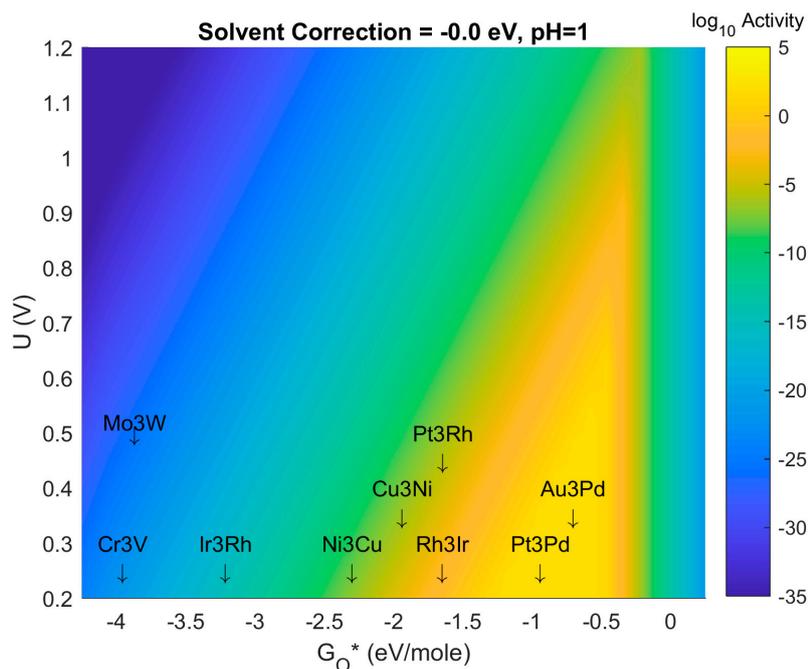
**Figure SI 3c.** Zoomed in From Figure 8 of Main Document Volcano Plot analysis for ORR activity at solvent correction value of  $-0.20$  eV. Top left (pH = 0), Top right (pH = 1), **Bottom left** (pH = 3), Bottom right (pH = 7). Blue denotes lowest activity, yellow denotes highest activity. All plots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



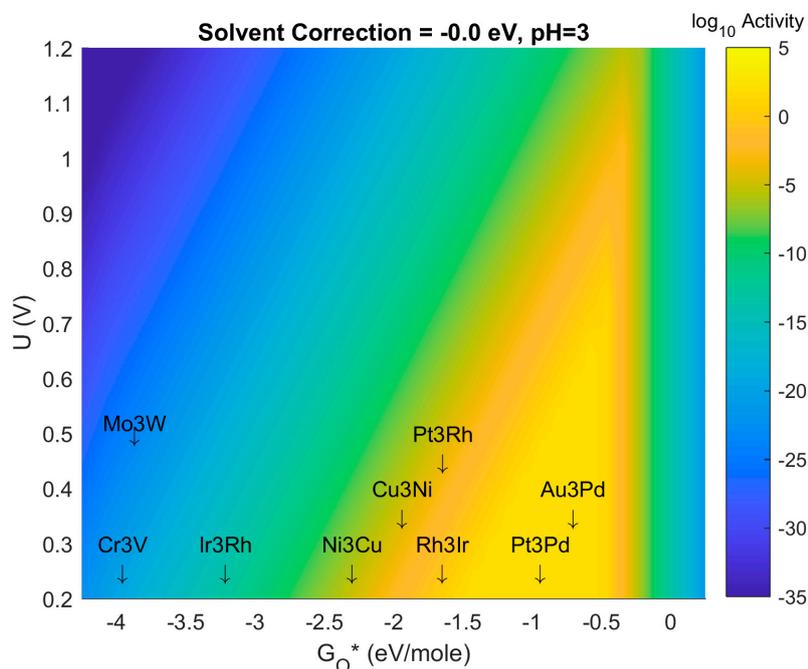
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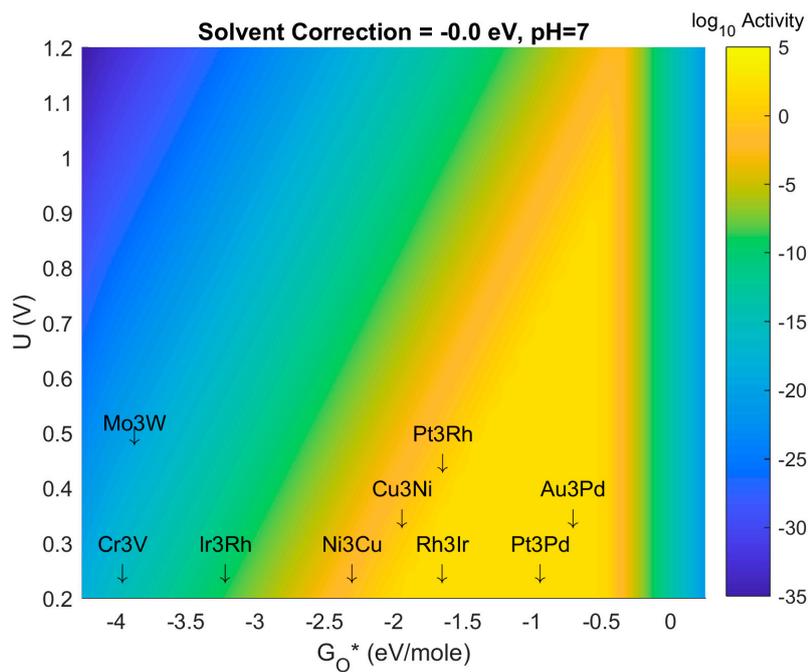
**Figure SI 4a.** Zoomed in From Figure 9 of Main Document Volcano Plot analysis for ORR activity at solvent correction value of  $-0.00$  eV. **Top left** (pH = 0), Top right (pH = 1), Bottom left (pH = 3), Bottom right (pH = 7). Blue denotes lowest activity, yellow denotes highest activity. All plots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



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