Analyzing Hydrogen Adsorption on Alloy Surfaces to Aid in the Design of Catalysts for Energy Applications
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Catalysts can save energy...
Catalysts increase the rate of a reaction by decreasing activation energy. They are widely applicable, but the focus of our research is designing catalysts for energy applications e.g. H2 evolution (HER).

HER forms H2 by splitting H2O, creating clean & renewable energy.

Adsorption energies are used to design catalysts.
In designing catalysts for hydrogenation, hydrogen adsorption energy should be neither too high or too low.

Adsorption energies should be hydrogenation activation energy. Reaction by decreasing catalysts.

Single Atom Alloys
Previous studies show that catalytic performance can be improved by doping an active transition metal into an inert host metal.

Solving for hydrogen adsorption energies

Alloy surfaces

Density functional theory (DFT)
A computational quantum mechanical method used to study electronic structures.

VASP is a code that models materials at the atomic scale and implements DFT.

The trends in adsorption energies are unexpected...

We expect $E_1 \approx E_2 \approx E_3$. However, Tc and Fe fail to follow this and exhibit unexpected behavior.

When do the trends occur?

Nonmonotonic behavior is observed when $E_2$, $E_3$, and/or $E_3 \neq 1$.

Are the trends only seen when Ag is the host?

Nonmonotonic behavior is also seen in other hosts such as Au, Cu, and Pd.

Are these trends related to density of states?

Density of States of Single Dopant on Ag Host

Patterns in density of state data relate to the nonmonotonic behavior observed.

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Conclusions
• The alloy surfaces studied demonstrate unexpected behavior that may provide new opportunities in catalyst design.
• This behavior is related to the density of states.

Cu, Ni, and Pd show what we expected:
• A monotonic change in $E_{ads}$ as the number of dopants increase
• $E_{ads}$ of sublevel doped catalysts to be about the same as isomers
Tc and V do not.

Are the trends only for reactions with H?

We are currently working on performing calculations for reactions with oxygen and reactions with carbon.