

1. What is the parameter that the study employs to judge the efficiency of catalyst?

Hydrogen adsorption energy.

2. What are the parameters used to probe the stability of the catalysts?

Four sets of parameters.

First, we estimate the free-energy change associated with surface segregation events; such events can cause surface solute atoms to segregate into the bulk.

Second, we determine the free-energy change associated with intrasurface transformations such as island formation and surface de-alloying.

Third, we evaluate the free energy of oxygen adsorption, beginning with splitting of liquid water; facile oxygen adsorption can lead to surface poisoning and/or oxide formation.

Finally, we estimate the likelihood that the surface alloys of interest will corrode in acidic environments (pH=0). For this test, we simply take the free energies of dissolution as reported in the electrochemical series.

3. What is the winning material?

PtBi

4. What impressed you most in this study?

Prediction; high throughput screening

5. Why should the parameter in 1 work?

Because hydrogen atom adsorbed on catalyst surface is the only intermediate. The adsorption energy should be not too high, nor too low.