Machine learning study of single-atom platinum supported on graphene (SAC-Pt-G) for fuel cell electrocatalysis

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Purpose Determining novel SAC-Pt-G and nitrogen-doped SAC-Pt-G structures using a global optimization-based structure search, then assessing the stability and reactivity of selected candidates

Contents
- Structure search produces different candidates of SAC-Pt-doped armchair and zigzag graphene nanoribbon and SAC-Pt-doped nanoflake
- Density functional theory (DFT)-based stability analysis to determine most stable candidates at different carbon terminations and hydrogen concentrations
- DFT-based adsorption study of OH, CO, and other ORR and CO oxidation intermediates
- Analysis of N-doped structures

Results

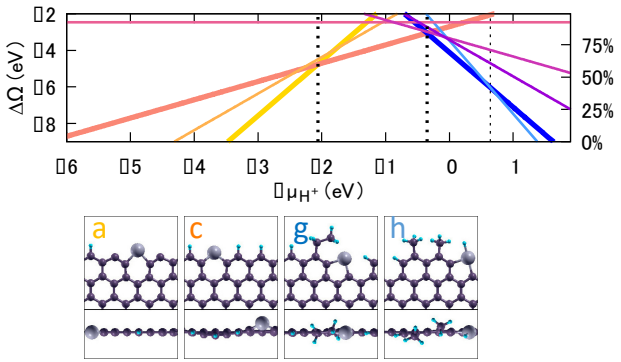
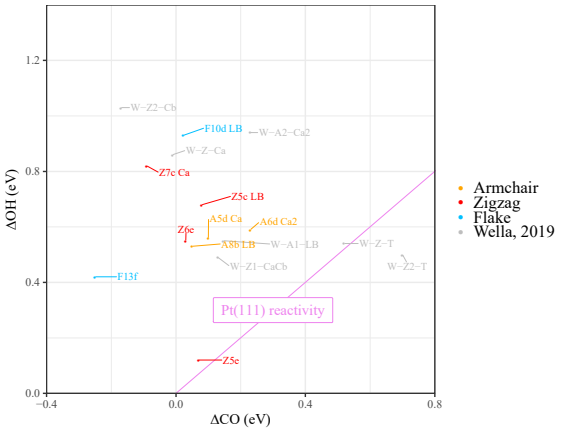
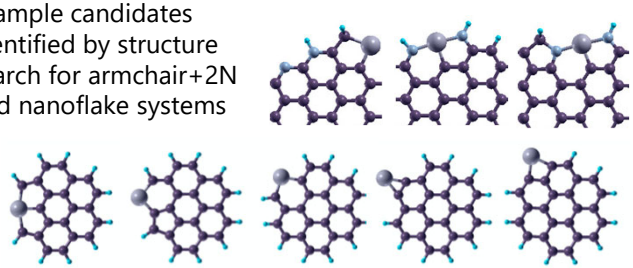


Figure 1. Phase diagram of formation energy versus hydrogen chemical potential, indicating stable structures obtained for zigzag nanoribbon SAC-Pt-G with a single vacancy.

Figure 2. OH vs. CO adsorption on selected candidates. These are compared to Pt(111), and the upper left region indicates favorable high OH and low CO adsorption.



Example candidates identified by structure search for armchair+2N and nanoflake systems



Computing system	SQUID
Node-hours	12,000
Memory	90 GB
Parallelization	76 CPU