

## Nanographene Catalysts for the Oxygen Reduction Reaction

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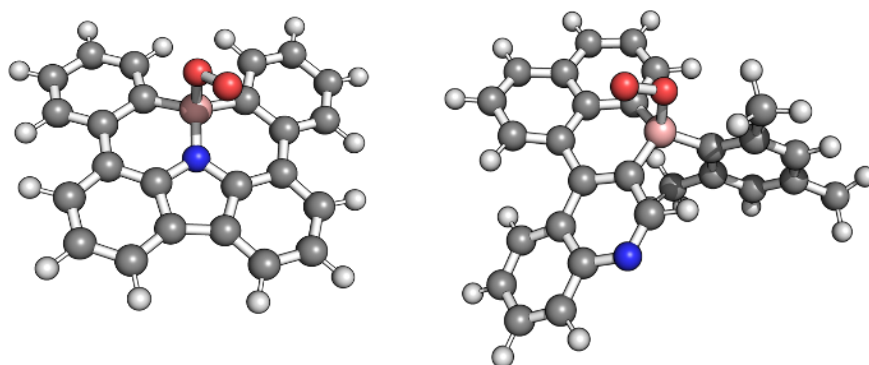
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The Oxygen Reduction Reaction (ORR) is an electrochemical process important in fuel cells and metal-air batteries. The bare reduction shows a rather sluggish reaction kinetics requiring catalysts to achieve larger electrical currents. Precious metal Pt-alloys show good performance and serve as a reference; however, their rareness, high prices and poor long-term durability inhibit large scale applications. Recently, a set of well-defined heteroatom-doped polyaromatic hydrocarbons have been reported as ORR catalysts [1], displaying a range of activities despite their structural similarity. To explain this observation and deduce the design criteria for nanographene ORR catalysts, we investigate the reaction pathway from the physisorbed oxygen towards the chemisorbed minimum by density functional theory [Figure 1]. We find that the initial chemisorption occurs *via* negatively charged catalysts, which is confirmed by exergonic reaction energetics. Electron affinity arises as a simple indicator of how likely an electron is to be transferred from the charged electrode to the catalyst. Beyond the experimentally reported systems, the electron affinities of several other polyaromatic hydrocarbons are partially correlated with their catalytic activities, therefore putting forward the electron affinity as an insightful descriptor for subsequent rapid catalyst pre-screening [2].

### References

- [1] R. J. Kahan, W. Hirunpinyopas, J. Cid, M. J. Ingleson, R. A. W. Dryfe, Chem. Mater., 31 (2019), 1891.
- [2] C. Ehlert, A. Piras, J. Schleicher, G. Gryn'ova, *in preparation*.

### Figures



**Figure 1:** Oxygen physisorbed on nanographene catalysts.