Termination Effects of Pt/*v*-$Ti_{n+1}C_nT_2$ MXene Surfaces for Oxygen Reduction Reaction Catalysis

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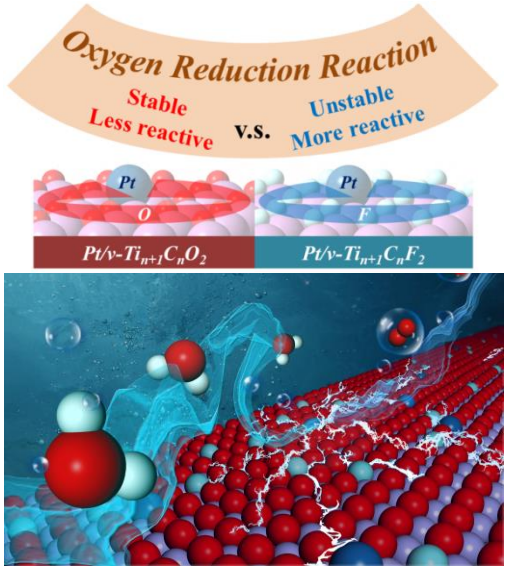
Ideal catalysts for the oxygen reduction reaction (ORR) have been searched and researched for decades with the goal to overcome the overpotential problem in proton exchange membrane fuel cells. A recent experimental study [1] reports the application of Pt nanoparticles on the newly discovered 2D material, MXene, with high stability and good performance in ORR. In this work, we simulate the $Ti_{n+1}C_nT_x$ and the Pt-decorated Pt/*v*-$Ti_{n+1}C_nT_x$ (n = 1−3, T = O and/or F) surfaces by first-principles calculations. We focus on the termination effects of MXene, which may be an important factor to enhance the performance of ORR. The properties of different surfaces are clarified by exhaustive computational analyses on the geometries, charges, and their electronic structures. The free-energy diagrams as well as the volcano plots for ORR are also calculated. On the basis of our results, the F-terminated surfaces are predicted to show a better performance for ORR but with a lower stability than the O-terminated counterparts, and the underlying mechanisms are investigated in detail. This study provides a better understanding of the electronic effect induced by the terminators and may inspire realizations of practical MXene systems for ORR catalysis.



Scheme1. The oxygen reduction reaction (ORR) on the Pt decorated O- and/or F-terminated MXene surfaces in an aqueous system.

References

1. Xie, X.-H.; Chen, S.-G.; Ding, W.; Nie, Y.; Wei, Z.-D. *Chem. Commun.* **2013**, *49*, 10112-10114.
2. Khazaei, M.; Ranjbar, A.; Arai, M.; Sasaki, T.; Yunoki, S. *J. Mater. Chem. C* **2017**, *5*, 2488-2503.
3. Liu, C.-Y. and Li, E. Y. *ACS Appl. Mater. Interfaces* **2019**, *11*, 1638-1644.