Modulating Catalytic Activity using a Ferroelectric

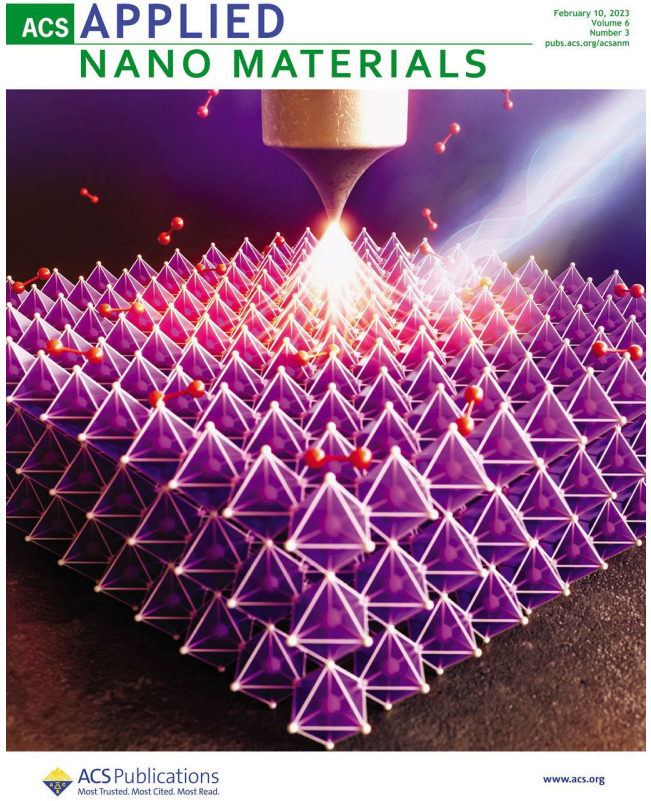
T.A. Pascal and D.P. Fenning (UC San Diego),
D.G. Schlom (Cornell), and V. Rose (Argonne National Laboratory)

Ferroelectric materials are widely utilized in nonvolatile memory, sensors, and actuators. But as a PARADIM user has recently demonstrated, the switchable structure at the surface of a ferroelectric can alter its electronic and interface properties—providing an excellent opportunity to modulate catalytic activity.

With the help of PARADIM, Fenning's group at UCSD has explored the use of MBE-grown epitaxial thin films of $BaTiO_3$—a ferroelectric model compound—to study the role of polarization on the hydrogen evolution reaction (HER) by surface spectroscopy and *ab initio* DFT+U calculations [1]. The work indicates that an upward-polarized (001) surface reduces the work function relative to the downward polarization leading to a smaller HER barrier, in agreement with higher catalytic activity observed experimentally.

To further elucidate the effect of polarization switching on surface structure and chemistry the researchers teamed up **with scientists from Argonne National Lab** to study the $BaTiO_3$ thin films by synchrotron X-ray scanning tunneling microscopy (SX-STM), a unique method that integrates nanoscale surface imaging and chemically sensitive spectroscopy [2].

In combination with *ab initio* calculations a stronger binding strength of a model reactant (here O_2) to the upward-polarized surface is observed. The work advances the understanding of the surface chemistry and electronic structure of ferroelectrics.



[1] P. Abbasi, *et al.* *Nano Letters* **22**, 4276-4284 (2022).
[2] P. Abbasi, *et al.* *ACS Applied Nano Materials* **6**, 2162-2170 (2023).
Access to data: 10.34863/80nw-gm95.