

Abstract Submitted  
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**Acceleration of non-PGM Electrocatalyst Design For Fuel Cells  
Through Site Specific XPS Predictions from First-principles Simulations**

BORIS KIEFER, New Mexico State University, SADIA KABIR, KATERYNA ARTYUSHKOVA, PLAMEN ATANASSOV, University of New Mexico — One of the most pressing problems in the 21<sup>st</sup> century is the provision of environmentally consistent energy technologies especially for space limited non-stationary applications. Fuel Cells are promising candidates for addressing and mastering this challenge. Alternative materials to platinum catalysts which continue to attract significant attention are non-PGM FeN<sub>x</sub>/C based materials. The understanding of the geometry and chemistry of catalytically active defect moieties is a prerequisite for the rational improvement and design of non-PGM electrocatalysts. XPS, a widely used surface analytical technique, generally shows broad N1s peaks with abundance weighted contributions from every defect motif. Due to the lack of appropriate reference materials it is currently impossible to de-convolute the N1s peak into defect specific contributions. In order to remove this limitation we have performed density-functional-theory (DFT) based calculations for a variety of in-plane Fe-N<sub>x</sub> (x=2-4) defects. Using DFT we predict, for the first time, defect chemistry and geometry induced N1s binding energy shifts in these materials. In combination with our XPS experiments and catalyst performance we find that higher FeN<sub>3</sub> defect abundance correlates with improved catalyst performance.

Boris Kiefer  
New Mexico State Univ

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