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Living On The Edge

BORIS KIEFER, New Mexico State University

Computational Physics continuous to significantly advance our understanding of the natural world that surrounds us. However, and may be even more importantly is the observation that computational models have reached a degree of sophistication that provides them with predictive power and reliability which are prerequisites for the successful integration of these techniques into the exploration and design of novel materials. One such effort is the area of energy conversion technologies for non-stationary applications that reduce the emission of greenhouse gases and increase energy independence and security. Fuel cells are among the prime candidates for such a technology. However, overcoming the performance limiting sluggish oxygen-reduction-reaction (ORR) at the cathode and the replacement of expensive and rare platinum catalysts remain challenging. I will discuss our contribution to gain new and innovative insights for the design and the performance of alternative TM-N_x (TM=Fe, Co, Ni, x=2,4) derived catalysts. Chemically altered graphene serves as a model system for the density-functional-theory based exploration of the ORR on these catalysts in alkaline and acidic media and for comparison with available experimental results.