Abstract Submitted
for the MAR17 Meeting of
The American Physical Society

Combining first principles modeling, experimental inputs, and machine learning for nanocatalysts design FATIH SEN, SPENCER HILLS, ALPER KINACI, BADRI NARAYANAN, MICHAEL DAVIS, Argonne National Lab, STEPHEN GRAY, Argonne Natl Lab, SUBRAMANIAN SANKARANARAYANAN, MARIA CHAN, Argonne National Lab — Nanocatalysts are of technological and scientific relevance for a large variety of catalytic processes. Due to the diverse geometries and complex structure-activity relationships, computational modeling and machine learning techniques are helpful in order to sample configuration space, incorporate experimental information, and account for co-variations in stability and catalytic activity. We will discuss structural determination of Au and IrO2 nanocatalysts from single and multi-objective global optimization algorithms, using as inputs density functional theory (DFT) calculations [1], a combination of energetic and simulated pair distribution function (PDF) data, and a combination of energetic and activity objectives. DFT data from thousands of Au nanostructures are fitted using a genetic algorithm to a hybrid bond-order potential (HyBOP)[2], which is able to predict structural and energetic properties of Au nanoclusters to bulk. Similarly, genetic algorithm is used to parametrize a variable charge potential for IrO2[3], which is instrumental in the combined multi-objective optimization of stability and activity. [1] A. Kinaci, et al, Sci. Rep. 6, 34974 (2016). [2] B. Narayanan, et al, J. Phys. Chem. C 120, 13787 (2016). [3] F. G. Sen, et al, J. Mater. Chem. A 3, 18970 (2015).

Maria Chan
Argonne Natl Lab

Date submitted: 11 Nov 2016 Electronic form version 1.4