Abstract Submitted
for the MAR08 Meeting of
The American Physical Society

Development of the relativistic tight-binding model for Platinum

ALEXANDER TCHERNATINSKY, J. WOODS HALLEY, University of Minnesota

— As a first step in a program to understand the mechanism of oxygen reduction on a platinum surface in an aqueous environment, we developed a relativistic self consistent tight- binding model for platinum. We applied a scheme that we successfully used previously for the description of titanium (S. Erdin, et al., PRB, **72**, 035405 (2005)) in which the electronic structure problem is described by an energy functional containing onsite terms depending self consistently on the local charge and interatomic terms. Due to the high atomic number of platinum, relativistic effects are known to be significant in the electronic structure. We include relativistic effects in the onsite functions of the tight binding model by making them self consistently dependent on the local Mulliken charge (as before) and also on the expectation values of the total atomic angular momentum number J of the atom and the occupation numbers of the $5d_{5/2}$ and $5d_{3/2}$ atomic orbitals in the tight binding basis. We find that this set of variables can uniquely describe the low energy states of the isolated platinum atom including relativistic effects. Their values are calculated self consistently in the tight binding model for the metal. The model was used to calculate the electronic structure of relaxed, low index platinum surfaces. Results will be compared with DFT results and with experiment. This work was supported in part by Minnesota Supercomputing Institute and U.S.DOE.

Alexander Tchernatinsky
University of Minnesota

Date submitted: 27 Nov 2007 Electronic form version 1.4