Applications of a Charge Transfer Formalism to the Design of Fuel Cell Materials

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Radical improvements in fuel cell performance are desired; therefore, extremely efficient electrocatalysts are essential to drastically improve over present systems. These improvements include the design of new catalysts and alternative fuels and electrolytes.

We present an ab initio procedure able to study materials at interfaces allowing their optimization. We apply the method to systems of interest for the development, study, and simulation of fuel cells. This procedure is based on density functional theory calculations of extended and molecular systems combined through a Green function approach to study charge transfer at interfaces. Applications of the method to known systems to evaluate the quality of the procedure will be followed by calculations on proposed, not yet used, materials.