Simulation web platform for electro-chemical oxygen reduction reaction

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Computer simulations of materials in atomic and electronic scale are widely used during the last few decades, yet, it is not easily applicable to majority of researchers. This difficulty is not only because of simulation theories to be learned but also because of preparing computer facilities necessary for the simulation and many other research skills to be familiar with. The simulation web platform we have developed recently is a good research equipment that solves this difficulties and allows researchers to focus not on the techniques to do researches but on their research target. In this presentation, we are going to demonstrate simulation platform for oxygen reduction reaction (ORR) in electro-chemical cell. The platform, named at qCat, has functions to build atomic structure of catalysts, analyzing electronic structures, calculating adsorption energies of chemicals and drawing reaction diagrams (Fig. 1). The qCat also provides simulation tools to find thermally stable atomic configurations of alloy particles (Fig. 2), and to test chemical stability by performing desolusion simulations. Density functional theory (DFT), molecular dynamics (MD), and Monte Carlo (MC) software are used behind the qCat along with postprocessing programs. Most of simulation parameters were preset and not shown to users so that they do not need to care about simulation techniques in detail. Using this qCat, even researchers who does not have an experience in simulations can do simulations for ORR by themselves, after just one or two days of practice.

ISBN 978-89-89453-30-7

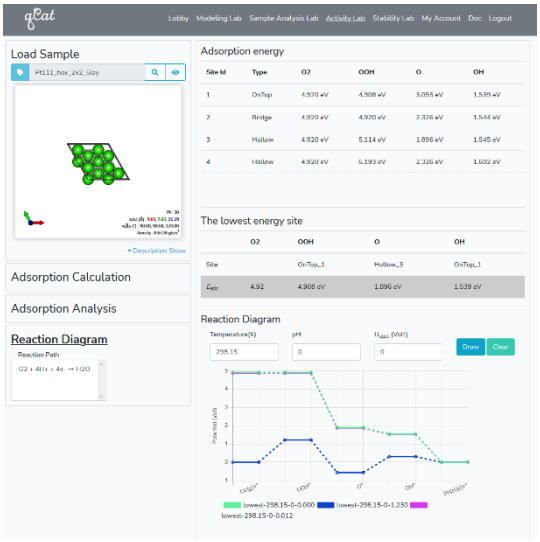

Fig.1: Activity test and reaction diagram of ORR in qCat. DFT calculations is used.

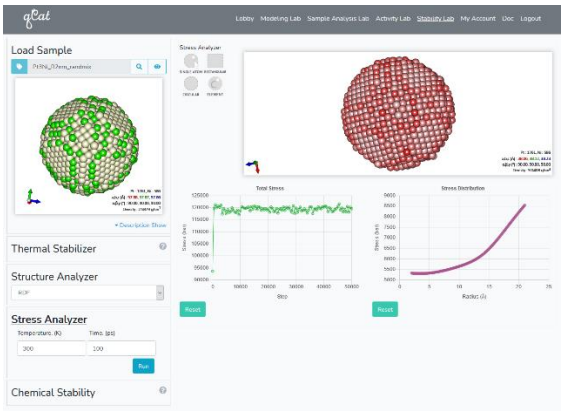

Fig.2: Thermally stable atomic configuration of Pt3Ni nano-particle and stress distribution calculated in the qCat. MC and MD simulations were performed with 2NNMEAM potential.

ISBN 978-89-89453-30-7