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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.

qCat		Lobby	Modeling Lab	Sample Ana	ysis Lab <u>Activity</u>	<mark>≀Lab</mark> StabilityLa	ib My Account	Doc Logout
Load Sample			Adsorption energy					
Pt111_hox_2x2_Slay	۹	0	Site Id	туре	02	OOH	0	он
			1	OnTep	4.920 eV	4.908 eV	3.055 eV	1.539 eV
			7	Bridge	4.920 eV	4.970 eV	2.326 eV	1.544 eV
			з	Hollow	4.920 eV	5.114 eV	1.896 eV	1.545 eV
1888A			4	Hollow	4.920 eV	5.193 eV	2.326 eV	1.602 eV
A sheet	4: 543, 54 9000, 9010	Pt: 30 1,31,29 1,29,89	The lowes	st energy s	ite			
*De	w.y. 860	Syn"		02	00Н	0	0	4
			Site		OnTop_1	Hollow_3	0	Top_1
Adsorption Calculation			L _{ads}	4.92	4.908 cV	1.896 eV	1.9	539 eV
Adsorption Analysis			Peaction (Diagram				
Reaction Diagram		Temperature	=(K)	рН	U _{uppi} (Volt)			
			298.15		0	0		Draw Clear
02 + 411+ + 4e- → 1120 ^			4	-				
				_			<u>\</u>	
			lowest-	1977 Iowest-298.15- 298.15-0-0.01	0-0.000 lowe	st-298.15-0-1.230	29200	r



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

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