EMMC case study:

Predicting the Oxygen-Binding Properties of Platinum Nanoparticle Ensembles by Combining High-Precision Electron Microscopy and Density Functional Theory

Interview of Dr Misbah Sarwar, Johnson Matthey

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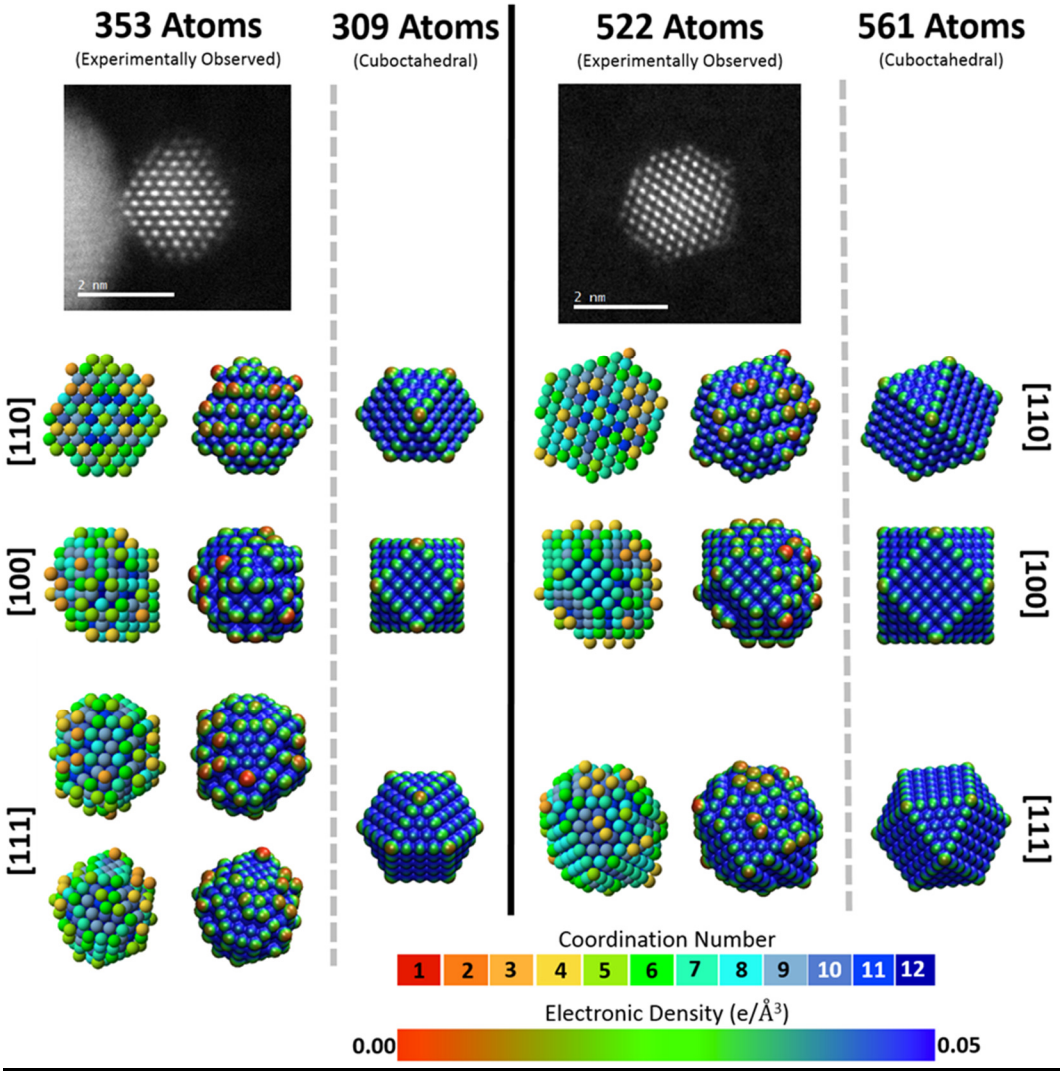


About the Company

Johnson Matthey (JM) is a global leader in sustainable technologies and employs 14000 people across 30 locations worldwide. 1450 of these people work in R&D. 20% of JM's research effort goes into central research, and the remaining 80% being spread across their

businesses in cleaning the air, making more efficient use of natural resources, and improving health.

In 2004, JM established a computational chemistry group resourced with hardware (e.g. a cluster) and software. While the focus of this group is on discrete modelling, continuum modelling has also been used in other parts of the company for about 25 years. Counting both the members of the discrete and continuum modelling groups, about 50 scientists across JM have relevant modelling experience that can be called on.

JM prefers to hire modellers with a PhD and provides internal and external continuous professional development. The group started with two modellers and now has nine dedicated modelling experts. Staff across other disciplines are encouraged to run routine calculations such as optimisations or NMR parameters, whereas the computational chemistry group tends to focus on cutting edge science – something which is very attractive to younger people looking to join JM's R&D teams. Besides the modelling, JM are looking at the use of AI and have hired data scientists to make sure the quality of the information is fit for purpose.

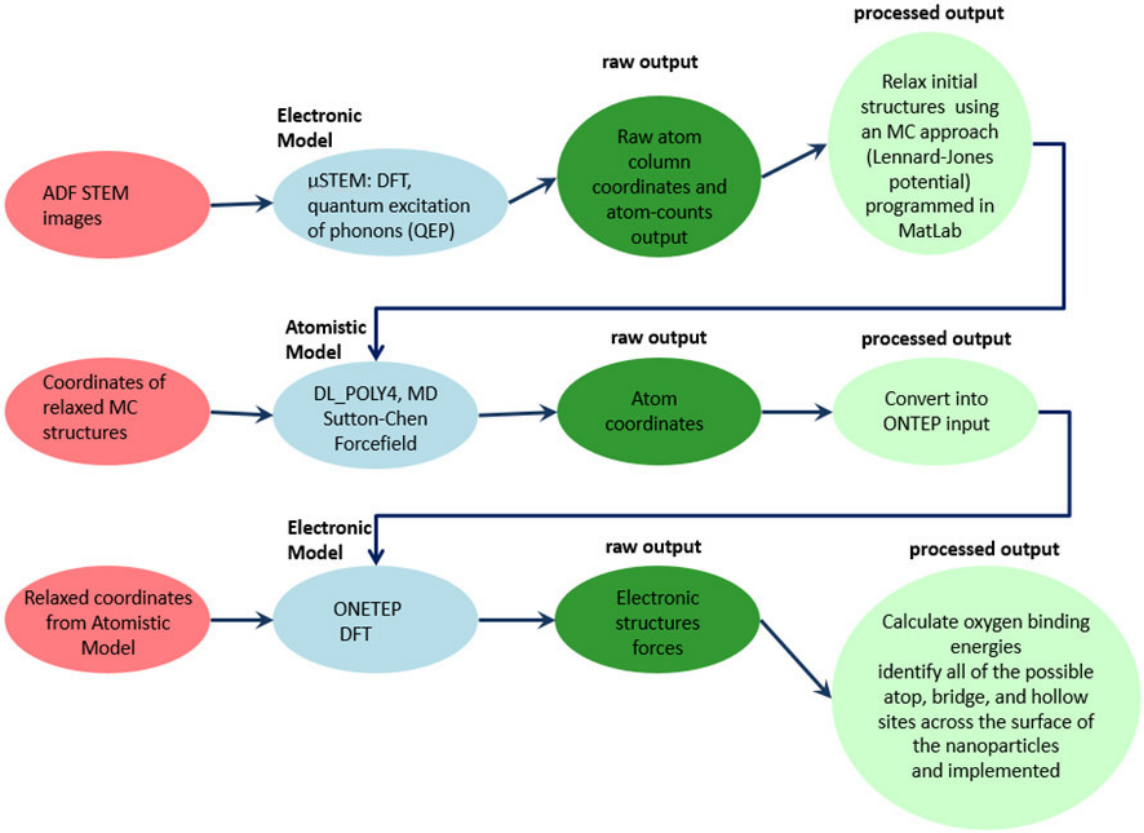
About modelling – the nuts and bolts

JM has expertise with electronic, atomistic, mesoscale and continuum modelling. Data-based modelling is used to close experimental gaps and they have a specialist in microkinetic modelling. They are also familiar with multiscale modelling and use model linking workflows, where data are passed from atomistic to mesoscale models, and results from electronic models feed into their microkinetic models. The computational group use coupled electronic/atomistic modelling, such as QM/MM. JM's experts use modelling continuously in their day-to-day work and are comfortable with both free/open-source and commercially supported software. The computational group comprises individuals with translator experience, so they can use different types of modelling for different applications/problems, always offering modelling where it will derive the most value.

JM's modelling team are highly self-sufficient and undertake most of their work in-house only needing occasional consultancy or training from a software vendor. A good network with academia means they can offer fellowships, explore new ideas/approaches to problems, acquire of new modelling expertise, access resources as needed (software, hardware) and strengthening the collaborations with academic institutions.

About the Case Study

The case is based on JM research into fuel-cell cathodes. It has been published in: "Predicting the Oxygen-Binding Properties of Platinum Nanoparticle Ensembles by Combining High-Precision Electron Microscopy and Density Functional Theory", J. Aarons, L. Jones, A. Varambhia, K.E. MacArthur, D. Ozkaya, M. Sarwar, C.-K. Skylaris, P.D. Nellist; Nano Lett. 17 (2017) 4003−4012 (DOI: 10.1021/acs.nanolett.6b04799)



For this particular case, which were your objectives as an industrial consumer of modelling?

JM wanted to consider the morphological diversity in real commercial product used in fuel-cell cathodes. The nanoparticles sit on support materials, which can change the morphology of these particles and lead to changes in adsorption capabilities which are relevant for the catalytic activity.

So, the modellers took a successful workflow based on an idealised model and made it more realistic. The idealised model does not include information of the nanoparticle size and their morphological variability, whereas the new approach can determine the optimum particle size to minimise detrimental surface roughness and particle shape effects.

How did materials modelling play a key role in problem solving?

JM wanted to generate a better model for nanoparticles. The commonly used model to study oxygen reduction reaction (ORR) catalysts would be to generate slabs under periodic boundary conditions (i.e. extended surfaces) that mimic a face of the nanoparticle. This is a very useful approach; even though it makes only use of idealised structures it still allows a decent screening for the ORR activities of a compound. The calculations can aid in finding descriptors that can be related to adsorption energies. Electronic-density values for each binding site in a nanoparticle (atop, bridge, or hollow) are used as descriptors of O binding strength, providing linear relationships for each binding energy as a function of the electron-density value. One advantage of such electronic descriptors is that they are expected to apply also to alloyed nanoparticles, for example.

What tools and methodologies have been applied?

Electron microscopy was used as an experimental pre-processing tool to get more realistic input coordinates for the nanoparticles. For the actual calculations, electronic models (CASTEP, ONETEP) and atomistic models (DL_POLY4) were used.

What were the expected improvements of the material behaviour simulation?

It was expected to bring more realism into the modelling.

For this particular case, did modelling affect your value chain?

Modelling could aid with understanding the properties of known materials better, as a combination of experiments and modelling allowed JM to investigate more realistic nanoparticles. Eventually, this will lead to a better understanding of the performance of a catalyst.

For this particular case, what was the quantitative value of materials modelling?

For this project, having higher quality data representing the material was key. The quantitative level is expected in the future as the new workflow promises better understanding.

What investments were made during the project?

JM shared the costs with their research partners. They financed two studentships comprising one experimentalist and one modeller. JM offered supervision and a travel budget for site visits.

For this particular case, how did you measure the impact of Materials Modelling as a tool to assist in problem solving, process optimisation, product development?

In JM material modelling is used routinely to solve specific problems so it is seen as a valuable asset. Performing experiments alone for this case was not sufficient, as one cannot decouple the individual factors contributing to an effect. Hence, JM decided to utilise materials modelling. The expected impact was the insight that modelling delivers which cannot be gained by experiment.

What technical and technological benefits resulted from the project?

In future, the new modelling workflow is expected to be used for more complex problems.

What were the economic benefits/impacts when you did use modelling?

The modelling workflow will lead to better screening of the catalytic activity of nanoclusters, and thus provide more reliable results. This has the benefit that promising materials can be found faster.

What was the business impact versus previous approach?

The new approach delivers more complexity and more realism, so predictions will be more sophisticated and JM can realise the catalytic potential of a materials more accurately.

Did modelling improve your competitiveness/innovation power?

The introduction of realism to a materials representation is seen as very innovative.

What sort of obstacles or barriers did you have to overcome to use modelling?

JM are pursuing improvements and overcoming barriers continuously. For this case, the modelling team reached out to their academic network to access additional expertise. The previous approach to model oxygen binding properties (simple surface slabs) was seen as sufficient but limiting. Thus, JM sought to overcome the limit through the use of modelling.