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An Overview of Modelling at Johnson Matthey

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Over the past fifteen years or so, the number of modellers at Johnson Matthey has grown from one, to close to twenty; a firm indication of the importance that JM places in both atomistic, as well as meso/macroscale modelling. DFT modelling in particular, forms an integral part of JM's research and development efforts in a wide range of areas, including catalysis, diagnostic services, pharmaceutical applications, and new battery and fuel cell technologies. The presentation will provide a brief overview of modelling at JM, highlighting the types of calculations that we do (with some real world examples), how modelling fits in with our experimental research programmes, the HPC resources that we utilize, and our interactions with the CHPC.

Presenter Biography

Primary author: Dr PERRY, Chris (Johnston Matthey)Presenter: Dr PERRY, Chris (Johnston Matthey)Session Classification: HPC Applications

Track Classification: Materials Science