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Investigation of oxygen adsorption on Pt nanoparticles with large-scale DFT calculations ALVARO RUIZ-SERRANO, PETER CHERRY, CHRIS-KRITON SKYLARIS, University of Southampton — The oxygen reduction reaction (ORR) is of central importance to the operation of fuel cells. An understanding of the chemistry of the adsorption of oxygen on the metallic surface of the cathode electrode, which is one of the stages involved in this reaction, can be acquired through ab initio calculations based on Density Functional Theory (DFT). The use of metallic nanoparticles can improve the performance of fuel cells, so it is important to understand how their material, shape, surface and size affect their chemical properties. However, traditional DFT approaches for metallic systems have constrained the investigations to a small number of atoms. Our recent developments within the ONETEP program for large-scale DFT calculations enable us to study much larger metallic systems consisting of hundreds or even thousands of atoms. In this work we use such calculations to perform a study of oxygen adsorption on platinum nanoparticles of a range of sizes, and examine properties such as the optimized structures, electronic effects and adsorption energies.

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