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MAX Phases as an Electrocatalyst Support Material: A DFT Study

The global increase in energy demand is causing increasing interest to be shown in the field of renewable energy. One of the potential new methods of green electricity generation is the hydrogen fuel cell. This uses hydrogen and oxygen to create electricity, with only water as a reaction product. However, before it is commercially viable, an issue of catalyst support material durability needs to be solved. Currently, carbon black is predominantly used to support platinum, but the carbon black oxidises under the conditions present in a fuel cell.

A new class of material has been developed within the last 20 years which displays properties that could be suitable for use in a hydrogen fuel cell. These new materials are a combination of ceramics and metals and are called MAX phases. Some MAX phases display good electrical conductivity and excellent oxidation resistance, which are the precise properties required to be a good electrocatalyst support material. Three of the most thoroughly studied MAX phases are Ti_3SiC_2, Ti_3AlC_2, and Ti_2AlC.

To determine which of these would be the most suitable candidate to use as an electrocatalyst support material, it is necessary to understand more about their properties. To do this, the MAX phases will be modelled using density functional theory (DFT), which can give insight into both molecular and bulk properties of a material. The primary properties that are going to be investigated are the electrical conductivity and the oxidation resistance. DFT calculations will be conducted on the CHPC using the molecular modelling program VASP (Vienna *Ab-initio* Simulation Package).

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