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DFT study of CO Oxidation by Molten Carbonate[1] SUSAN NJOKI, CHANGYONG QIN, GODWIN MBAMALU, Benedict College — In the past years, molten carbonate (MC) has been adopted to solid oxide fuel cells (SOFCs) as booster for the oxygen reduction process in the cathode. The reaction pathway through CO42- as reaction intermediate has been revealed by DFT modelling. Simply, CO42- is a carbonate ion with atomic oxygen attached and it has very strong oxidizing capacity, implying a possible novel catalyst for various oxidization reactions at high temperatures. In this study, we have investigated the CO oxidation by MC using DFT methods. Two reaction intermediates, C2O42- and C2O52-, are formed by CO with CO32- and CO42-, respectively. The activation energy is calculated to be 10.0 kcal/mol through a Langmuir-Hinshelwood mechanism. In addition, the interactions between Nitroxides (NOx) and MC were examined because NOx has been proven as a poisoning gas for many industrial catalysts. This study confirms that NO will react with CO42- to form NO2, and NO2 will then leave MC. No poisoning was found by the DFT modelling, which implies that MC can be potentially used for CO oxidation in the exhaust gas treatment of combustion engines.

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