Predicting Chemical Reaction Equilibria in Molten Carbonate Fuel Cells via Molecular Simulation

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In the electrolyte of a molten carbonate fuel cell there are a number of reactions that can occur which lead to the formation of undesired species, such as hydroxide ions. Since the molten salt electrolyte is present at extreme temperatures, it is challenging to measure its composition experimentally. Therefore, using molecular simulations, we have computed the composition of hydroxide in several molten alkali carbonate salts as a function of water and carbon dioxide partial pressures. The results reveal that there can be a substantial concentration of hydroxide in the melt at low partial pressures of CO_2. In addition, the equilibrium concentration of molecular water dissolved in the electrolyte is found to be over two orders of magnitude higher than that of CO_2 over a wide range of partial pressures. Increasing the size and polarizability (or in other words reducing the “hardness”) of the cations can reduce the hydroxide fraction, but at the cost of lowering ionic conductivity.