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Developing Iridium-based Alloys as Effective Catalysts for Direct Ethanol Fuel Cells[1] LIDA NAMIN, AARON DESKINS, Worcester Polytechnic Institute, KORETAKA YUGE, Kyoto University, KYOTO UNIVERSITY COLLABORATION — Fuel cells enable the conversion of different chemicals directly into electrical energy, and are much more efficient than conventional combustion engines. Direct ethanol fuel cells (DEFCs) use ethanol as a fuel source. However, DEFCs are not commercialized due to the lack of an efficient catalyst. Iridium alloys are promising catalysts as they possess high catalytic activity and are much cheaper than platinum, the traditional fuel cell catalyst. Synthesizing all possible alloys experimentally is a burdensome task which is not economically feasible. As a result, in this study we have developed realistic atomic models of iridium alloys in DEFCs. Since density functional theory (DFT) methods are limited by finite computation power, we used the combination of DFT with statistical physics methods, specifically, cluster expansion (CE). Our results show how theoretical methods can advance alloy development by predicting stable structures of iridium alloys.

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