Showcasing research from the Computational Materials Design Group (CMDG), Discipline of Chemistry and Center for Material Science and Engineering, Indian Institute of Technology Indore, India.

Single-layered platinum nanocage: a highly selective and efficient catalyst for fuel cells

A stable single-layered octahedral platinum nanocage (Pt$_{66}$) has been predicted using density functional calculations. The nanocage is very efficient and selective towards four-electron oxygen reduction reaction (H$_2$O formation) over two-electron oxygen reduction reaction (H$_2$O$_2$ formation). Therefore, the product selectivity (H$_2$O vs. H$_2$O$_2$) is excellent compared to any catalysts reported to date. Thus, we predict that the single-layered nanocage could be a promising catalyst for fuel cell applications.

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