

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_2O formation) over two-electron oxygen reduction reaction (H_2O_2 formation). Therefore, the product selectivity (H_2O vs. H_2O_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.



