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Rational design of competitive electrocatalysts for the oxygen reduction reaction in hydrogen fuel cells SERGEY STOLBOV, University of Central Florida Physics Department, MARISOL ALCÁNTARA ORTIGOZA, Karlsruher Institut für Technologie, Institut für Festkörperphysik, Karlsruhe, Germany — The large-scale application of one of the most promising clean and renewable sources of energy, hydrogen fuel cells, still awaits efficient *and* cost-effective electrocatalysts for the oxygen reduction reaction (ORR) occurring on the cathode. We demonstrate that truly rational design renders electrocatalysts possessing both qualities. By unifying the knowledge on surface morphology, composition, electronic structure and reactivity, we solve that sandwich-like structures are an excellent choice for optimization. Their constituting species couple synergistically yielding reaction-environment stability, cost-effectiveness and tunable reactivity. This cooperative-action concept enabled us to predict two advantageous ORR electrocatalysts. Density functional theory calculations of the reaction free-energy diagrams confirm that these materials are more active toward ORR than the so far best Pt-based catalysts. Our designing concept advances also a general approach for engineering materials in heterogeneous catalysis.

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