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DESIGN OF NOVEL ELECTROCHEMICAL CATALYST CONFIGURATIONS FOR CARBON DIOXIDE CONVERSION FOR EARTH AND OUTER SPACE APPLICATIONS

Abstract

For achieving sustainability and closed-loop strategies in the framework of value-added fuels and oxygen supply for onsite energy generation, spacecrafts propulsion, breathable atmosphere and CO2 emissions reduction, whether on Earth or for future space missions, performance and cost challenges need to be addressed. Among the most promising alternatives considered so far, electrochemical catalysis for CO2 reduction reactions has the potential to serve as a viable solution due to its engineering and economic feasibility, with the possibility of controlling the reactions by altering the electronic structures, the surface geometry parameters and the applied voltage; nevertheless, key obstacles remain because of its high temperature and pressure requirements. This raises the need to design optimal electrocatalysts to boost CO2 conversion performance, under ambient environment with very low input voltage. A desirable reaction rate can be realized by controlling the surface and interface atomic arrangement, which maximizes the adsorptive sites for reactants and intermediates and simultaneously minimizes the adsorptive sites for spectators and products. Based on the desired products, different parameters can be optimized depending on the considered catalysts. For instance, nanostructured faceted catalysts with high surface energies are beneficial for improving the performance, a large variety of Pt- and Pd-based nanocrystals enclosed within high-index lattice plane can significantly enhance the activity and stability, while Cu can exhibit high reaction rates and capable of producing C1–C3 hydrocarbons. Metallic particle size has an optimum that must be considered, very small particles perform hydrogen evolution reactions over the CO2 reduction reactions, while Au nanoparticles with an optimal size can provide more edge sites than corner sites, which is advantageous to CO formation. Also, nitrogen-doped graphene-like materials coated on conducting polymer electrodes can show good results for CO2 conversion to CH4 in ionic liquids. Cu nanoparticle cluster-based metal organic framework can achieve high performance for CH4 production; while similar results with nitrogen and boron-doped single-walled carbon nanotubes, or boron and nitrogen co-doping method can be obtained for oxygen reduction reactions and hydrogen evolution reactions. Ni supported on SiO2–Al2O3 substrate can also reach very high selectivity for CO2 conversion. The current approach aims, first, to establish an evaluation system for electrocatalytic performance assessment based on the state-of-the-art of recent work carried out to date, then, to theoretically and numerically investigate the most relevant configurations, and finally, to classify and screen the optimal electrocatalysts in terms of engineering and economic feasibility.