Title

Axiomatic Design of a PhotoElectroChemical Cell for Ethylene Production

Authors

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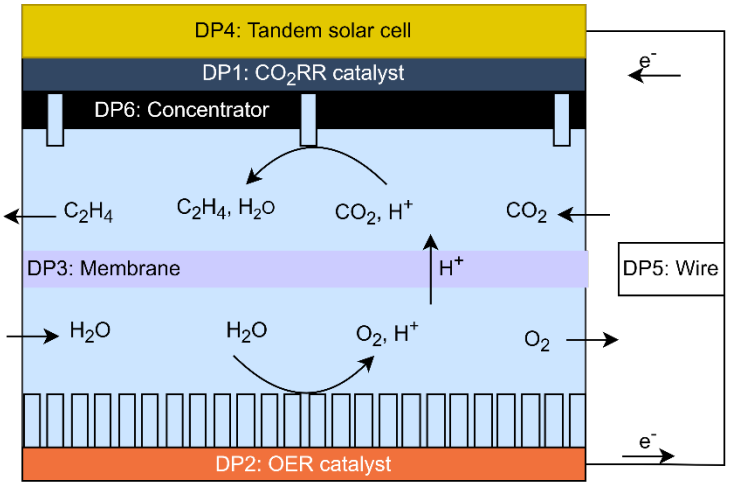
Abstract oral / poster presentation (*please choose your preferred means of presentation*)

To set up a rational and robust engineering theory for developing a device to photosynthesize ethylene (C_2H_4) from water and CO_2 with an optimized photon-to-product yield, we utilize Axiomatic Design (AD). In contrast to the current practice of combining two interdependent modules, a photoanode and a photocathode, we specify a decoupled design with six design parameters. Our design starts with selecting the CO_2 reduction reaction (CO_2RR) catalyst, followed by the oxygen evolution catalyst and the proton-transporting membrane. Next, the tandem solar cell should provide the required potential at high photogenerated current densities, and an electron-transporting wire is necessary. Finally, concentration is required to enable high selectivity towards ethylene. To create a robust solar to ethylene design that is insensitive to environmental fluctuation of the light intensity, the selected CO_2RR catalyst should display high selectivity towards ethylene over a broad range of current densities. Production rates up to 31.3 μmol/cm^2/h ethylene, corresponding to a solar-to-ethylene efficiency of 11.6%, are calculated for O(II)D-Cu as CO_2RR catalyst combined with $NiFeO_x$ as OER catalyst and coupled to tandem solar cells with bandgaps of 1.90 and 1.35 eV. In our simulation the CO_2RR is sparsely applied to the solar cells to achieve concentration of current on the catalyst, which is necessary to optimize the performance. In addition, this configuration is able to operate with high yield and selectivity over a wide range of solar irradiation conditions. Alternative ways to achieve the required concentration include adding a sixth module that concentrates sunlight to boost carrier production for driving CO_2 reduction in a PEC cell setup, or carefully aligning the potential and current densities between the photovoltaic and electrochemical parts in a photovoltaic electrochemical cell (PV-EC) configuration.



References (*max 3*)

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