Comprehensive Description of Transport Phenomena in Soap-film Functional Membranes

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We here investigate a pioneering concept in the realm of renewable energy: soft, self-assembled photosynthetic membranes for the photocatalytic conversion of carbon dioxide into fuel. These novel membranes utilize soap films integrated with functional molecules, aiming to harness solar energy effectively. Our approach encompasses a comprehensive multi-scale and multi-physics modeling framework, designed to theoretically analyze and optimize this new concept. At the macroscale, the model describes the transport of gaseous and ionic species within the soap film, detailing the chemical equilibria and the dual photocatalytic half reactions of CO_2 reduction and water oxidation at the gas–surfactant–water interfaces. The mesoscale model, utilizing Monte Carlo simulations, delves into the structural morphology of the functional monolayers. This dual-module approach facilitates a nuanced understanding of the membrane's operation under various conditions, significantly contributing to the design of efficient solar fuel production systems. Key findings include the critical influence of electron relays, buffer concentration, and CO_2 pressure on fuel production. Our parametric analysis identifies optimal conditions for maximized CO yield, particularly highlighting the significance of photosensitizer-to-catalyst ratios and buffer concentrations. This research underscores the importance of understanding the interplay between charged species at the interface and the resultant effects on fuel production efficiency. While promising, our study acknowledges the limitations due to the current gaps in fundamental and experimental knowledge of these systems. It serves as a foundational step towards possible future refinements of soft photosynthetic membranes and encourages further investigation using techniques like neutron scattering, sum frequency generation spectroscopy, and time-resolved spectroscopy. Ultimately, this work can pave the way for future advancements in photocatalytic technologies and the broader application of such membranes in various photochemical reactions.