Quantum Computational Models for Photoelectrochemical

Processes in Solar Fuel and Energy Conversion Systems

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***Abstract*—Quantum computational models are emerging as powerful tools for understanding and optimizing photoelectrochemical (PEC) processes that underpin next-generation solar fuel and energy conversion systems. These systems involve complex interactions between photons, charge carriers, catalytic surfaces, and molecular intermediates, making accurate predictive modeling challenging for classical simulation frameworks. This study investigates quantum-enabled approaches for simulating light–matter interactions, exciton dynamics, charge-transfer pathways, and catalytic reaction coordinates within PEC architectures. By leveraging quantum algorithms for electronic structure, nonadiabatic dynamics, and reaction energetics, the research explores how quantum simulations can resolve strongly correlated states, multi-electron excitations, and interfacial charge separation with higher fidelity. The analysis highlights the potential of quantum models to accelerate the discovery of efficient photoelectrode materials, enhance solar-to-fuel conversion efficiencies, and support the rational design of artificial photosynthesis systems. Finally, the paper discusses the integration of quantum computational predictions with experimental PEC workflows and outlines opportunities for future hybrid quantum–classical research.**

The global shift toward sustainable energy has intensified interest in photoelectrochemical (PEC) systems capable of converting sunlight into chemical fuels. These technologies, including water-splitting devices, CO_2 reduction platforms, and solar-driven hydrogen production systems, rely on a sequence of highly intricate processes: photon absorption, exciton formation, charge separation, catalytic activation, and multi-step reaction pathways at semiconductor–electrolyte interfaces [1]. Capturing the full complexity of these interactions in a single theoretical framework remains challenging due to the simultaneous presence of quantum-scale electronic behavior, mesoscale transport phenomena, and multi-electron catalytic mechanisms [7].

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Traditional computational chemistry methods provide important insights but often struggle to describe strongly correlated electrons, excited-state dynamics, interfacial charge-transfer events, and the nonlinear coupling of electronic and nuclear degrees of freedom that define PEC efficiency [5]. Quantum computational models offer a transformative alternative by enabling a more accurate representation of many-body electronic states and the energetics of photochemical reactions. Through quantum algorithms tailored for electronic structure, excited-state evolution, and nonadiabatic transitions, researchers can explore processes that are

