Multiscale and multiphyiscs modeling and simulation of proton transport through membrane proteins

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Proton transport is one of the most important and interesting phenomena in living cells; it plays many crucial roles in biological processes such as cellular respiration, ATP synthase, and cancer cell development. Due to special properties of protons and membrane channels, traditional convection-diffusion models are not suitable to study proton flux; quantum dynamics is instead adopted. However, extremely expensive computational costs are required for a full quantum model. The present work proposes a multiscale/multiphysics quantum dynamic in continuum model for proton transport through membrane proteins, in order to balance physical accuracy and simulation efficiency. The current model is in form of total energy framework, from which governing equations are derived. Advanced mathematical tools are developed to handle the challenges in simulations and validity of the proposed model is verifed through comparison of the simulations and experimental data.