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Abstract for an Invited Paper
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Development of effective models for vectorial biological processes[1]

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Progress towards understanding vectorial processes in biological systems using theoretical and computational approaches will be discussed. The specific problems of interest include mechanochemical coupling in the molecular motor myosin and vectorial proton pumping in cytochrome c oxidase. Several related methodological developments will be discussed, which include boundary potential for QM/MM simulations, effective QM methods for treating long-range proton transfers and phosphate chemistry, and coarse-grained models for describing large-scale motions in biomolecules. Quantitative benchmark calculations of these methods have been carried out using both model and realistic biological systems. The application of these methods to myosin and cytochrome c oxidase will be briefly presented.

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