

Insights: Publications

Editors' choice—review—exploration of computational approaches for understanding microbial electrochemical systems: opportunities and future directions

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Microbial electrochemical systems offer valuable opportunities in the field of electrochemistry for a wide range of applications and fundamental insights. Applications include renewable power generation, electrosynthesis, and sensing, and provide a critical platform for understanding fundamental electrochemical processes between biotic and abiotic components. However, despite several research efforts, the fundamental electron transfer mechanisms inherent to microbial bioelectrochemical systems remain poorly understood, limiting their full potential and applications. This lack of fundamental understanding stems from both the conceptual and experimental complexity of microbial electrochemical systems. In this context, the possibility of multi-disciplinary research utilizing computational methods provides a powerful tool for this field. Herein, we critically review how computational studies and methods employed to study microbial electrochemical systems in multiple dimensions can be used to clarify the different factors governing microbial electrochemical systems. This discussion addresses how the combination of various techniques can enhance fundamental understanding, providing scientists with tools for the rational design of improved systems and opening exciting new research opportunities.