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Computational modeling of electron transfer in hydrogenase and carbon material complexes KWISEON KIM, HAI LONG, National Renewable Energy Laboratory — In biohybrid and biomimetic devices for energy conversion, the electron transfer between the enzyme and the electrode plays a central role. We use hydrogenase and carbon material as model systems and investigate the binding and electron transfer configurations between hydrogenase and carbon materials, including single-wall carbon nanotubes and graphene surfaces. We use Brownian dynamics simulations to sample the hydrogenase/carbon material phase-space. The results provide an atomistic picture of how enzyme interacts with the electrode materials. We find that the optimal enzyme/electrode binding configurations are not optimal for electronic tranfer.

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