

'Global Simulations' in Photo-electro-catalysis: A Tribute to Enrico Clementi and Robert Cave

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Global Simulations and parallel processing were two visionary and transformative ideas that emerged through Enrico's career. In a tribute to Enrico, we will highlight the underlying and enduring frameworks in these areas, and how they have still a growing influence in the field of computation and simulation. Inspired by the 'global simulation' model, we will then discuss our recent research dealing with the multi-facets of charge generation, transport, and reactivity in photo-electro-catalysis for water oxidation, using first-principles methods and first principle-informed kinetic Monte Carlo modeling. As we discuss charge carrier transport, this presentation will also pay a tribute to Robert Cave, a giant in electron transfer theories and methods.