Theoretical and computational methods and models will be developed to study excitation energy transfer in photosynthetic light harvesting chromophore arrays. In these systems excitons move in coherent multi-chromophore quantum superposition states, with essentially no loss over large distances depositing their energy into reaction centers where transformation and storage are initiated. Experiments suggest this quantum coherent energy transmission is due to correlated motions of the nano-structured proteins housing the chromophores. Large-scale classical simulations will be conducted to parameterize multi-state quantum system - bath models whose coherent quantum dynamics can be studied with new mixed quantum-classical methods. The lessons learned about controlling coherent quantum dynamics will find applications in designing next generation hybrid solar cell materials, and may guide the way towards controlling decoherence with applications in quantum information.

This new simulation methodology will be applied to study experiments in two areas: (1) In collaboration with the Toronto group of Scholes, calculations will be carried out for comparison with their experiments to explore the dependence of multichromophore network energy transfer efficiency on network geometry, environmental spectral density characteristics, chromophore electronic coupling, etc. The objective of these studies is to explore the design principles underlying natural photosynthetic light harvesting arrays. (2) The second application project, conducted in collaboration with the Dublin group of Thampi, involves constructing reduced dimensional models of harvesting networks coupled to DSSC materials to explore how interfacing biological light harvesting antenna networks with photovoltaic materials might be optimized to design highly efficient natural harvesting - synthetic transformation - hybrid materials.