In this work we demonstrate how quantum chemistry (QC) methods and molecular
dynamics (MD) simulations can be used in combination with Frenkel exciton model (FEM)
to obtain optical and excitation energy transfer properties of complex molecular systems
from the molecular structure. The combination of QC and MD methods with FEM provides
a powerful tool to study and explain molecular level processes, which are out of reach of
the standard FEM parametrization. We use these methods to study and explain molecular
mechanism of excitation energy transfer in rylene dyads, especially to explain observed
fast excitation energy transfer in dyad with orthogonal arrangement of transition dipoles,
where standard approach predicts no excitation energy transfer. On a fundamental level,
we relate FEM to configuration interaction method of QC and propose extension of FEM,
which accounts for interaction between excitonic manifolds. We investigate effects of this
interaction on the optical properties. Inspired by the core features of FEM, we propose
new concept of artificial light harvesting antenna based on fluorographene, with design
principles inspired by natural light harvesting complexes. We use structure based methods
to investigate its excitation transfer properties. We also introduce a new general method
for treating environmental effects on excited state properties of embedded systems, which
can be used as an extension of widely used polarizable QM/MM approach.