Learning about molecular excited states from high-throughput calculation: discovery and insight

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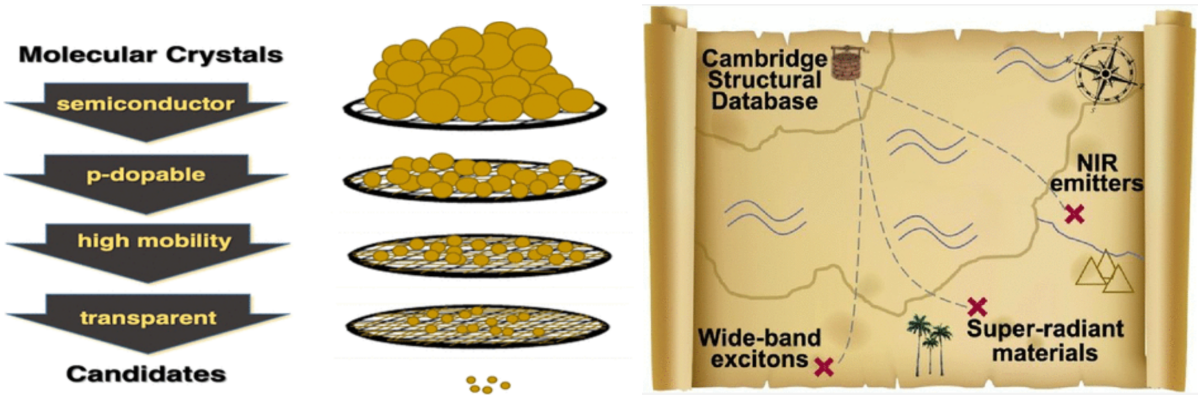
This talk will explore the interplay between detailed models, reduced model and high-throughput virtual screening to achieve useful generalizations in the area of organic electronics. Computational detailed model can be deployed to derive simplified modesl or to explore vast chemical space. Both approaches can be seen as different routes to achieve global understanding of phenomena and class of materials. The talk will consider excitons in solid, singlet fission, temperature activated delayed fluorescence, colour purity and non-radiative transition. It is shown that a vast array of phenomena can be tackled with the same approach. Our platform for the discovery of organic electronics materials is also presented with emphasis on the approach we follow to remove the barrier between physical prediction and experimental verification.



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