Executive Summary Report of

MINOR RESEARCH PROJECT
No: **2368-MRP/15-16/KLMG002/UGC- SWRO**

"Large-scale ab initio calculation for Designing Efficient Organic Molecules for Application in Organic Light Emitting Diodes (OLEDs) and Dye Sensitized Solar Cells (DSSCs)"

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By

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Large-scale ab initio calculation for Designing Efficient Organic Molecules for Application in Organic Light Emitting Diodes (OLEDs) and Dye Sensitized Solar Cells (DSSCs).

Organic molecules play a key role in many devices for energy conversion, particularly those where light is involved. For example, in the new generation of display screen equipment and energy-efficient lighting – organic light-emitting diodes (OLEDs) – the use of organic molecules as phosphorescent emitters allows large gains in efficiency through the harvesting of otherwise wasted triplet states. Meanwhile, in the reverse process of light-to-electrical energy conversion, organic molecules that absorb light to generate charge-transfer states are at the forefront of research into dye-sensitised solar cells (DSSCs). All of these applications require certain properties of the organic molecule to be optimized.

In this project we have used large scale ab initio quantum chemistry calculations on the singlet and triplet energy levels of several anthanthrene derivatives generated by the substitution of large number of conjugated and aromatic systems at 4,10/6,12 positions. We find that the peripheral functionalization on the anthanthrene core doesn't affect its frontier molecular orbitals, however, both the singlet and triplet energies can vary. The energies of the S_1 and T_1 states obtained are such that all the molecules could potentially be a TTA candidate. Properties of Anthanthrene derivatives such as high molar light absorptivity, reasonably long lifetimes of the S_1 and T_1 states and fluorescence emission quantum yields makes them attractive candidates for both SF and TTA applications. We expect the molecules could potentially be used in these applications.