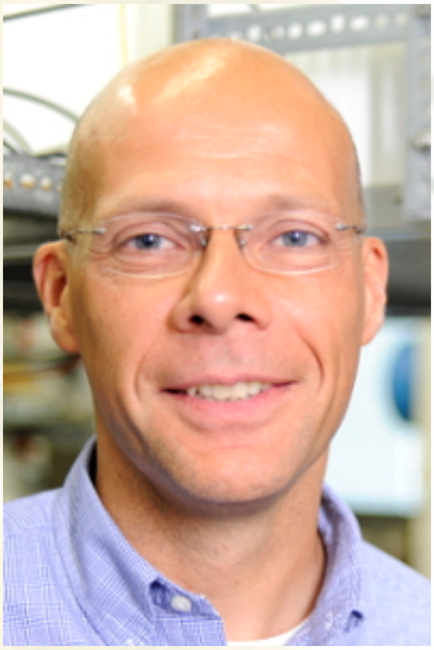
TOR VERGATA

UNIVERSITÀ DEGLI STUDI DI ROMA

Dipartimento di Scienze e Tecnologie Chimiche

PhD degree in Chemical Sciences

Honorary Doctorate



Towards breaking the barrier to 100% charge transfer

Dirk Guldi

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Aula Gismondi
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The Philosophy Doctor degree in "Chemical Sciences" is pleased to award the Honorary Doctorate to Dirk Guldi for his contribution to a novel vision of the nature of molecular and nanostructured systems.

His investigations of novel chemical and light driven nanostructures, open the way to the development of optimized materials for solar energy conversion devices.

Towards breaking the barrier to 100% charge transfer

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Chemistry affects almost every aspect of our existence, so that it will be an essential component of solutions in global issues in health, materials, and energy. For this reason, the design and synthesis of novel molecular materials lies at the forefront of transformative research and has game-changing character. A leading example for such shifts in existing scientific paradigms is surpassing the Shockley-Queisser limit, which places an upper bound on solar conversion efficiency for a single p-n junction solar cell at slightly more than 30%, by means of singlet fission (SF) in molecular acenes, the molecular analog to multiple exciton generation (MEG). In an optimal SF process, the lowest singlet excited state of one molecule (S_1) that is positioned next to a second molecule in its ground state (S_0) is down-converted into two triplet excited states (T_1) each residing on one of the two adjacent molecules. The two triplet states initially form a correlated pair state $^1(T_1T_1)$, which then evolves into two separated triplet states ($T_1 + T_1$). As such, the energetic requirement for SF is $E(S_1) \geq 2 \times E(T_1)$. Shifting the focus to intramolecular SF in dilute solutions rather than intermolecular SF in crystalline thin films enabled important breakthroughs.