

Abstract Submitted  
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**Evidences for Ti-N anchoring in organic dyes on TiO<sub>2</sub> and its influence on photovoltaic performance**<sup>1</sup> YANG JIAO, SHENG MENG, Inst. Physics, Chinese Academy of Sciences, SEEC LAB TEAM — New metal-free organic dyes with a novel donor-pi-acceptor design produce efficiencies exceeding 10% for dye-sensitized solar cells (DSSC) applications since 2010. Based on state-of-the-art electronic structure calculations and real time time-dependent density functional theory (TDDFT) simulations, we present consolidated evidences for novel Ti-N anchoring at the interface for such a broad group of new dyes, inferred from energetics, vibrational recognition, and electronic and optical data. This fact is contrary to what people usually believed and assumed in previous experiments and was largely ignored. We further demonstrate that the presence of interface Ti-N bonds largely benefit the electronic level alignment and photoelectron injection dynamics, greatly contributing to the improved efficiencies of DSSC based on cost-effective, environment-friendly organic dyes.

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