Excitonic properties of Titania

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Although titanium dioxide (TiO_2) is widely employed in fields like photovoltaics and photocatalysis, the nature of its fundamental charge transfer excitations is still unclear. A deep understanding of the excitonic properties of TiO_2 is of high relevance to achieve major advances in the aforementioned fields and may lead to the fabrication of new devices with enhanced performance in energy conversion applications. In my talk, I will present our most recents findings on the excitonic characteristics of both the rutile and anatase polymorphs of TiO_2, using state-of-the-art theoretical calculations and advance steady-state and ultra-fast spectroscopies. I will show that for anatase, the direct optical gap is dominated by a strongly bound exciton with a two-dimensional character [1]. Possible connections between the nature of this exciton and the enhanced photocatalytic activity of the anatase TiO_2 (001) facet will be discussed. Importantly for light-energy conversion applications, I will show that our results also apply to defect-rich samples. Control and modulation of the excitonic features via its interaction with phonons will also be explored [2, 3]. Finally, I will address an observed anomaly in the temperature dependence of the excitons in both the rutile and anatase polymorphs. [4]

[1] Strongly bound excitons in anatase TiO2 single crystals and nanoparticles. E. Baldini, L. Chiodo, A. Dominguez, et al. *Nat. Commun.*, 2017, **8**, 13.
[2] Phonon-Driven Selective Modulation of Exciton Oscillator Strengths in Anatase TiO2 Nanoparticles. E. Baldini, T. Palmieri, A. Dominguez, P. Ruello, A. Rubio, and M. Chergui. *Nano Lett.*, 2018, 18(8)
[3] Exciton Control in a Room-Temperature Bulk Semiconductor with Coherent Strain Pulses. E. Baldini, A. Dominguez, et al. Sci. Adv., 2019, 5(11)
[4] Anomalous anisotropic exciton temperature dependence in rutile TiO2. E. Baldini, A. Dominguez, et al. *Phys. Rev. B*, 2017, **96**, 041204(R).