# SEMINARIO


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# *Defect-induced charge transport, excitonic and magneto-optical properties of van der Waals interfaces from first principles.*


**Abstract:** The study of charge transfer, magneto-optical and excitonic properties of van der Waals matter has been the subject of intense research in recent years due to the importance of these materials for ultrathin optoelectronic, photovoltaic and photocatalytic components. In such applications, quasi-particles and excitons, often act as carriers in charge, spin and energy transfer processes, which can be significantly impacted by structural complexity, reduced dimensionality, interface composition or the presence of impurities and adatoms.
In this talk, I will address some of these complexities from first principles, focusing on transition-metal dichalcogenides (TMDC) and TMDC-graphene interfaces.
I will discuss the role of state localization due to atomic-size defects on the optical and magnetic properties [1, 2]. Using many-body perturbation theory, I will show how the excitonic picture associated with the presence of defects, can lead to structurally controllable excitonic magnetic response [3]. I will delve into the role of symmetries in charge transfer and excitonic properties on TMDC-graphene heterobilayers with monoatomic chalcogen vacancies. I will analyze the impact of the subgap defect-based features on the microscopic dynamics and excitonic features. Finally, I will show how defects can become a slow coherent transport channel for interlayer charge transfer [4] while simultaneously stronlgy altering the exciton properties of the TMDC-graphene interface due to a combination of folding, screening and mixing of the optical transitions [5].



[1] E. Mitterreiter, B. Schuler, A. Micevic, D. Hernangómez-Pérez, et al. Nat. Comm. 12, 3822 (2021).
[2] T. Amit, D. Hernangómez-Pérez, G. Cohen, D. Y. Qiu, and S. Refaely-Abramson, Phys. Rev. B 106, L161407 (2022).
[3] A. Hötger, T. Amit, J. Klein et al. npj 2D Mater. Appl. 7, 30 (2023).
[4] D. Hernangómez-Pérez, A. Donarini, and S. Refaely-Abramson, Phys. Rev. B 107, 075417 (2023). Editors' Suggestion.
[5] D. Hernangómez-Pérez, A. Kleiner, and S. Refaely-Abramson (arXiv:2303.13650).


**Sala de Seminarios B-118, Departamento de Física Teórica, Atómica y Óptica**
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