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Simulating hot carrier relaxation in materials: from bulk to low dimensional systems

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Abstract

Light matter interaction is of utmost importance in a number of technological applications. In photovoltaics, the excitation of carriers is a key ingredient. It leads to the formation of excitons, which are strongly bound in low dimensional systems, and the dynamics of carriers upon excitations if energy harvesting is possible.
In this talk I will discuss some recent developments in our group regarding optical excitations and the dynamics of hot carriers in several scenarios. I will discuss the formation of strongly bound excitons in van der Waals materials with possible applications in photovoltaics. Furthermore, for the case of Tellurene I will present work on ab initio calculated hot carrier lifetimes [2]. This is done using a combination of density functional theory, density functional perturbation theory, GW simulations and the inclusion of electron-hole correlations via the Bethe-Salpeter equation.
In the case of photocatalytic metals such as palladium and platinum I will discuss how direct optical transitions of photoexcited carriers in these metals are mainly generated in the near-infrared range. We also find that the electron-phonon mass enhancement parameter for Pt is 16% higher than Pd, a result that helps explain several experimental results. Finally, I will discuss how efficient hot electron generation and extraction can be achieved in nanofilms of Pd and Pd cleaved in specific directions.

References

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[2] CEP Villegas, MS Leite, A Marini, AR Rocha, Efficient hot-carrier dynamics in near-infrared photocatalytic metals, Physical Review B 105, 165109 (2022).