# Ultrafast phonon-driven charge transfer in van der Waals heterostructures

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Transition metal dichalcogenides (TMDs) are characterized by enhanced light-matter and Coulomb interactions leading to a rich energy landscape of tightly bound excitons. Stacking TMD monolayers into van der Waals heterostructures enriches the scenario even more, introducing spatially separated interlayer states and adding another exciton species with long lifetimes and an out-of-plane dipole moment.
Recent experiments demonstrated an ultrafast charge transfer in TMD heterostructures. However, the nature of the charge transfer process has remained elusive. Based on a microscopic and material-realistic exciton theory, we reveal that phonon-mediated scattering via strongly hybridized intervalley excitons governs the charge transfer process that occurs on a sub-100fs timescale. We track the time-, momentum-, and energy-resolved relaxation dynamics of optically excited excitons and determine the temperature- and stacking-dependent charge transfer time for different TMD bilayers [1]. In a very recent joint experiment-theory study, the predicted two-step charge transfer process has been compared with time-resolved ARPES measurements (performed in the group of Stefan Matthias, Georg-August-University Göttingen) [2] showing an excellent agreement.
The provided insights present a significant step for a microscopic understanding of the technologically important charge transfer process in van der Waals heterostructures.

## References

[1] Meneghini, G, Brem, S, Malic, E., Natural Sciences (2022), 2.4: e20220014.
[2] Schmitt, D., Bange, J. P., Bennecke, W., AlMutairi, A., Meneghini, G., Watanabe, K., ... & Mathias, S., Nature (2022), 608(7923), 499-503.

## Figures

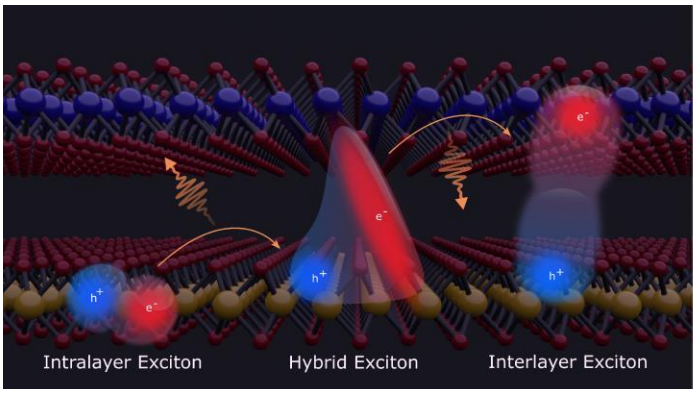


**Figure 1:** Sketch of the charge transfer process. Starting from an exciton localized in the bottom layer, phonon-mediated scattering to an hybrid exciton state (where e.g. the electron lives in both layers) allows for the transfer of the charge (here electron) to the upper layer resulting in a spatially separated interlayer exciton state.