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# ICFO researchers address long-standing debate in charge carrier transport

A team led by ICFO clarifies the transport mechanisms of charge carriers in MoSe<sub>2</sub>, identifying key parameters that influence their behavior in this atomically thin material, which is crucial for a range of optoelectronic devices.

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Transition metal dichalcogenides (TMDCs) are atomically thin semiconductors that are emerging as key components in a wide range of advanced technologies. They can be used in electronics as transistors, in optics as emitters and detectors, among various other applications. To keep advancing this type of technologies, a deep understanding of the underlying mechanisms that govern charge carrier transport is vital.

In recent years, numerous experiments have investigated the ultrafast transport properties of TMDCs, with a particular emphasis on their **diffusivity** (the rate at which particles spread, usually moving from a region of higher to lower concentration). However, the proliferation of studies on this topic has led to a wide variety of apparently inconsistent results, giving rise to long-standing controversies that still persist today.

ICFO researchers **Dr. Giulia Lo Gerfo Morganti**, **Dr. Guillermo D. Brinatti Vazquez**, led by **ICREA Prof. Niek F. van Hulst**, in collaboration with the Universitat Marburg, the Catalan Institute of Nanoscience and Nanotechnology (ICN2) and Technical University Eindhoven, have recently shed some light on the issue. In a Nature Communications article, they introduce a systematic experimental study, supported by unifying microscopic model, of charge and energy transport in MoSe<sub>2</sub> (a TMDC). Their findings reconcile previously conflicting results by highlighting **two critical factors: the material's dimensionality** (the number of one-atom-thick layers) **and its interaction with the underlying substrate** (the material over which the sample is deposited).

## Overnight measurements bore fruit

To investigate these effects, the ICN2 team fabricated MoSe<sub>2</sub> samples of varying thicknesses -some as thin as a single atomic layer- and suspended them over a 15 micrometer-sized hole to study transport behavior in the absence of a substrate. Then the ICFO team used ultrafast laser pulses and time-resolved microscopy to track how charged carriers moved through the

material over time, ultimately retrieving transport properties like its diffusivity. Working with free-standing monolayers posed a major technical challenge due to their extreme fragility and weak optical response, which significantly complicated data collection. We overcame this by conducting extended overnight measurements, repeating the experiments across multiple sample regions, and rigorously analyzing the data to ensure an accurate interpretation, shares Dr. Giulia Lo Gerfo Morganti, ICFO researcher and first author of the article. These precautions were essential for generating reliable, high-quality results, although they significantly extended the timeline of the project, she adds. In the end, the team discovered that monolayer, free-standing MoSe<sub>2</sub> exhibits extremely fast charge carrier diffusion compared to multilayer and substrate-supported layers, and that at this ultrafast diffusion collapses after approximately 1 picosecond (10<sup>-12</sup> seconds). Moreover, the material's thickness and the presence/absence of a substrate strongly influence how the system reaches that collapse regime as well.

#### Benefits for optoelectronic devices

Our findings were supported by microscopic simulations developed in collaboration with Prof. Ermin Malic and Dr. Roberto Rosati at Universitat Marburg, comments Dr. Lo Gerfo Morganti. These simulations elegantly matched the experimental results, further confirming that both layer thickness and substrate coupling are fundamental parameters that govern transport mechanisms at the atomic and subatomic level. According to the researcher: **This insight is critical for optoelectronic applications, such as ultrafast photodetectors and efficient solar cells**, where precise control of charge carrier dynamics is essential for device performance and design. Looking ahead, the researchers plan to extend their approach to suspended monolayers of other TMDC materials, which could potentially reveal new emergent transport phenomena at the nanoscale. Our simulations are ready. Now we just need to see whether the corresponding experimental data matches them, concludes Dr. Lo Gerfo Morganti.

#### Reference:

Lo Gerfo Morganti, G., Rosati, R., Brinatti Vazquez, G.D. et al. Transient ultrafast and negative diffusion of charge carriers in suspended MoSe<sub>2</sub> from multilayer to monolayer. Nat Commun 16, 5184 (2025).

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