Band transport by large Fröhlich polarons in MXenes

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Abstract

MXenes are newly emerging layered two-dimensional materials with great promise for electrochemical energy storage and (opto)electronic applications.^[1] A fundamental understanding of charge transport in MXenes is essential for such applications, but has remained under debate. While theoretical studies pointed to efficient band transport^[2], device measurements have revealed thermally activated, hopping-type transport^{[3].}

Here we present a unifying charge transport picture in two model MXenes by combining ultrafast terahertz and static electrical transport measurements to distinguish the short- and long-range transport characteristics.^[4] We find that band-like transport dominates short-range, intra-flake charge conduction in MXenes, whereas long-range, inter-flake transport occurs through thermally activated hopping. Our analysis of the intra-flake, i.e., inherent charge transport, shows that carrier scattering is dominated by scattering from longitudinal optical phonons with relatively weak electron-phonon coupling (coupling constant $a \approx 1$) in MXenes. The weak electron-phonon coupling gives rise to the formation of large polarons in MXenes: electrons and holes locally deform the lattice, and are dressed by a lattice distortion extending over several lattice units. Our work provides insight into the polaronic nature of free charges in MXenes, and unveils intra- and inter-flake transport mechanisms in the MXene materials, relevant for both fundamental studies and applications.

Reference

[1] A. VahidMohammadi et al. Science 65, 372, eabf1581 (2021);

[2] Z. Jing et al. J. Phys. D: Appl. Phys. 54, 015301(2021);

[3] J. Halim, et al., Phys. Rev. B 98 104202, (2018);

[4] W. Zheng et al. Nat. Phys., in press (2022), https://doi.org/10.1038/s41567-022-01541-y.

Figures



Figure 1: Schematic of large polaron formation in MXenes following optical excitations.

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