Lattice dynamics and carrier transport in $HgPSe_3$ by THz time domain spectroscopy

F. Grandi[1,2], A. Baserga[1], S. Dal Conte[1], C. Vozzi[2], E. Cinquanta[2]
1 – Department of Physics, Politecnico di Milano, Milan, Italy
2 – CNR IFN – Istituto di Fotonica e Nanotecnologie, Milano, Italy

Abstract: In this work we exploited THz time resolved spectroscopy to investigate the interaction between low energy lattice dynamics and charge carrier transport in a bulk layered semiconductor: $HgPSe_3$.

In recent years, significant interest has emerged regarding a new class of layered van der Waals materials: the metal phosphorus trichalcogenides (MPX3). This attention stems from the momentum generated by graphene and transition metal dichalcogenides (TMDs), as MPX3 materials offer a way to overcome some limitations of TMDs [1].

Among this family, mercury phosphorus triselenide ($HgPSe_3$) stands out for its photoconductive performance, driven by a direct bandgap near 2.0 eV at room temperature positioning $HgPSe_3$ as a strong candidate for fast, broadband photodetectors [2]. Despite this potential, there is not yet a fundamental understanding of the material's ultrafast properties, particularly regarding the interaction between charge carriers and the low energy collective lattice dynamics, such as the shear and breathing modes of the layered structure.

In this work, we employ ultrafast Terahertz Time-Domain Spectroscopy (THz TDS) to investigate the microscopic scattering mechanisms governing charge transport and recombination in bulk $HgPSe_3$. With both static transmission and optical pump-THz probe experiments, we disentangle the interplay between low-energy vibrational modes and carrier conductivity.

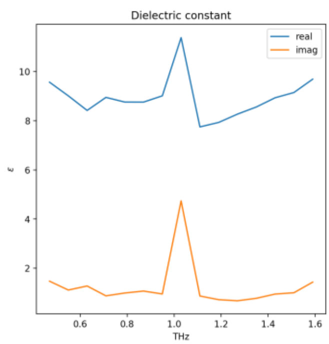

Fig.1 | Static dielectric constant of $HgPSe_3$

Static measurements in the 0.5–1.5 THz spectral window reveal distinct resonances identified as interlayer breathing and shear modes, Figure 1. Subsequently, time-resolved measurements probe the transient photoconductivity following ultrafast excitation. The spectral response reveals a complex conduction mechanism, characterized both by a Drude-like free carrier transport and strong localization effects driven by the coupling to the vibrational modes previously identified, Figure 2.

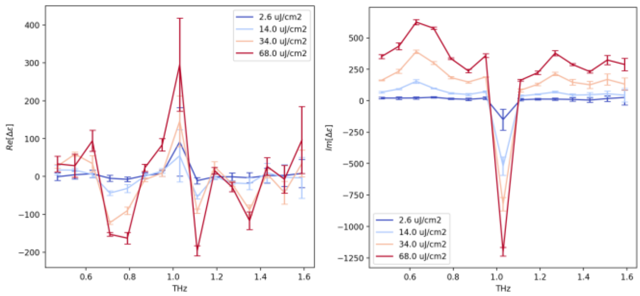

Fig.2 | Real and imaginary part of the transient dielectric constant at different fluences

This work's aim is to set a starting point over the study of such low energy vibrational modes and their interaction with the transport dynamics of layered semiconductors with the aim of improving their optoelectronic performance.

Contacts:

Federico Grandi (federico.grandi@polimi.it)

References

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