

Evidence of a two-step metallization process in transition metal dichalcogenides semiconductors under pressure

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Transition Metal Dichalcogenides (TMDs) are crystals characterized by a layered structure, with strong intra-layer covalent bonds and weak inter-layer van der Waals forces. The application of pressure provides an effective way to modulate the interaction between adjacent layers, allowing getting a deeper insight into the fundamental physics of these materials and paving the way for new applications in which the design of devices with tailored features is of utmost importance. Pressure-dependent studies have found that most of semiconducting TMDs undergo a pressure-induced transition toward a metallic state. However, a certain ambiguity still exists in the determination of the metallization pressure and in the explanation of the microscopic origin of the transition, as spurious effects related to the presence of disorder and intrinsic defects can lead to significant changes in the pressure response of the samples.

In this framework, we present a study of the high-pressure metallization in TMDs semiconductors by synchrotron-based infrared spectroscopy. The combined results from far- and near-infrared ranges gave us new insights into the mechanisms ruling the evolution of the sample electronic properties, indicating a metallic transition taking place in two steps: the first at lower pressure arising from the overlap between doping and conduction band states, the second at high pressure associated with the band-gap closure. The pressure response of the Fano resonance in the E_{1u} phonon, here reported for the first time, was exploited as spectroscopic benchmark to understand the doping-related electronic processes ruling the metallic transition.