Tunability of exciton and trion properties in monolayer and bilayer MoTe₂ encapsulated in various dielectric environment

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Molybdenum ditelluride (MoTe₂ is an indirect gap semiconductor in its 2H crystallographic form. It can be changed to direct gap material with the decreasing number of monolayers to a single one or two. The monolayer (ML) and bi-layer (BL) 2H-MoTe₂ direct-gap energy is established to ~1.10 eV (1125 nm) and ~1.05 eV (~1200 nm) at room temperature, respectively. Therefore, it makes the material attractive for light-emitting devices operating in the near-infrared spectral range.

Importantly, as in other 2D transition metal dichalcogenides, the Coulomb correlations between electrons and holes in 2H-MoTe₂ strongly determine the optical bandgap of the material and can be tailored through the screening of the Coulomb interaction by placing the material in the different dielectric environments.

This report explores this optical gap tuning possibilities in mechanically exfoliated ML and BL 2H-MoTe₂ exposed to a technologically relevant dielectric environment potentially vital for the fabrication of hybrid MoTe₂/classical semiconductor/insulator optical devices.

Optical properties of MoTe₂ are evaluated by high-spatially-resolved photoluminescence, differential reflectivity, photo-modulated reflectivity, and Raman studies at cryogenic and room temperature. Materials combination includes either typical ones: ML and BL 2H-MoTe₂ encapsulated in PMMA/air, SiO₂/air, hBN/air, SiO₂/hBN, hBN/hBN, Si/air, and Si/hBN interfaces, and less known: Si₃N₄/air, 4H-SiC/air, GaP/air, InP/air, GaAs/air, Si₃N₄/hBN, 4H-SiC/hBN, InP/hBN, and GaAs/hBN. Mentioned interfaces can be characterized by an effective electric permittivity ε_{eff} spanning the range of ~(2.0-9.85). The dielectric screening results in shifting the emission energy of exciton (X) and trion (T). We show that the dielectric screening, accompanied by the renormalization of a quasi-particle bandgap, only slightly influence the exciton emission energy (E_X) , showing its decreasing of about a few meV with increasing the ε_{eff} . A slightly stronger trend is observed for a trion for which the emission energy (E_T) can decrease by ~10 meV with increasing the $\varepsilon_{\rm eff}$. These observations are reflected in the tuning range of the trion binding energy: $E_{b,T} = E_X - E_T$. For ML MoTe₂, the $E_{b,T}$ can be tuned in the range of ~(26-22 meV), exhibiting distinct descendance with the ε_{eff} . The $E_{b,T}$ in BL MoTe₂ follows the same trend, however, showing a tunability range of ~(20-15 meV). These studies can be important for the design process of the ML or BL MoTe2 embedded optical cavity that must consider the dielectric screening within excitons and trions caused by the cavity material. In this respect, the cavity mode must be precisely aligned to the exciton or trion emission line.