Abstract

This dissertation thesis focuses on the study of mechanical and optoelectronic properties of 2D materials for solar energy conversion and their tunability through interaction with different types of substrates. The main goal is to describe how mechanical stress induced by various substrates affects the structural, optical, and electronic properties of graphene and transition metal dichalcogenides, particularly tungsten diselenide (WSe_2).

The first part of the thesis focuses on the characterization of Schottky contacts in 2D/3D heterostructures of graphene on a silicon substrate, the study of mechanical properties of graphene on flexible substrates, and the characterization of local deformation phenomena, such as the formation of wrinkles and folds, which affect the distribution and transfer of charge carriers, and, thereby, the performance of these structures in solar applications.

2D/3D heterostructures of exfoliated graphene transferred onto freshly etched n-doped silicon were characterized using two conductive atomic force microscopy (C-AFM) methods: local current-voltage (I-V) measurements and area-wide characterization using contact-mode C-AFM. These methods were complemented by pseudo-I-V curves, calculated from area-wide measurements. Photovoltaic parameters were further optimized by doping with $AuCl_3$, which significantly improves the electrical properties of the Schottky diodes, notably increasing short-circuit current and open-circuit voltage. The fill factor remains unchanged due to localized doping, which prevents a reduction in specific resistance.

The shape and formation of graphene wrinkles on SU-8 polymer were examined using AFM methods. The wavelength and amplitude of the wrinkles are proportional to the mechanical stress and thickness (number of layers) of graphene. Kelvin-probe force microscopy measurements demonstrate that the surface potential of wrinkled graphene is influenced more by the number of graphene layers than by its wrinkling, as graphene is supported by the polymer across its entire area, and surface variations in charge carrier concentration are negligible.

In the next section, monolayer transition metal dichalcogenides (TMDCs), particularly WSe_2, are further studied in relation to their strong interaction with gold substrates and subsequently as suspended (freestanding) membranes. Using AFM indentation, we deform the suspended WSe_2 membranes and tune their optical and electronic properties.

Selected TMDC materials (MoS_2, $MoSe_2$, WS_2, and WSe_2) were exfoliated onto a perforated, gold-coated substrate and characterized using Raman spectroscopy. While 3D materials and suspended monolayers show minimal shifts in Raman modes, gold-supported monolayers exhibit a shift in the E mode towards lower energies and splitting of the A_1 mode. These changes in vibrational properties are caused by the strong interaction between TMDC materials and gold, as well as the tensile stress that gold exerts on the material. This effect

is less pronounced in the selenides due to the smaller difference between their lattice parameters and gold. Additionally, the E'' and A_2'' modes, otherwise forbidden in suspended monolayers, become active in Raman spectroscopy when the TMDC materials are supported by gold.

Suspended monolayers of WSe_2 were subjected to the first comprehensive study combining AFM tip-induced nanoindentation with *in-situ* measurements of photoluminescence emission and generated photocurrent. The values of the Young's modulus ranging from 160.1 to 164.5 GPa are consistent with the literature and MD simulations. The highest stress that the suspended WSe_2 can withstand was determined to be ≈30 N/m. Measurements and analysis of force-distance curves highlight the importance of using a combination of a second independent method, in this case, photoluminescence, to accurately determine the onset of indentation and correctly calculate the mechanical properties. The increasing photocurrent values, in contrast to dark currents that remain negligible even with increasing indentation, evidence the presence of a photo-induced effect, where the carrier flow is aided by the local deformation of the WSe_2 in the vicinity of one of the contacts (the AFM tip).