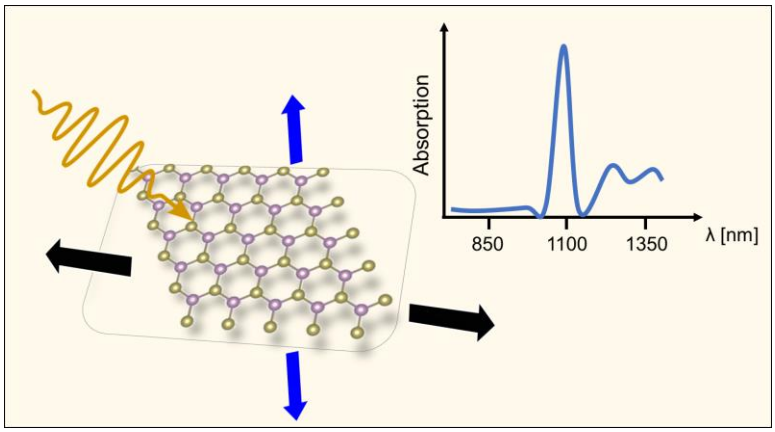
Potential of strained monolayer $MoTe_2$ and its vdW heterostructures as photon absorbers in the telecom range

Muhammad Sufyan Ramzan[1] **and Caterina Cocchi** [1,2]

[1]*Institut für Physik, Carl von Ossietzky Universität, 26129 Oldenburg, Germany.*
[2]*Center for Nanoscale Dynamics (CeNaD), Carl von Ossietzky Universität, 26129, Oldenburg, Germany.*

To exploit the full potential of two-dimensional (2D) materials and their van der Waals heterostructures (vdW HS), it is essential to understand and rationalize the interplay between their structural and electronic properties. Using density-functional theory, we investigate the impact of uniaxial strain on the electronic and optical properties of monolayer $MoTe_2$ [1]. Considering both compressive and tensile strains up to ±10% along the armchair and zigzag direction of the 2D sheet, we examine how the fundamental gap, the band dispersion, the frontier states, and the charge distribution are modified. Under tensile strain, the system remains a semiconductor, but a direct-to-indirect band gap transition occurs above 7%. Compressive strain, instead, is highly direction-selective. When it is applied along the armchair edge, the material remains a semiconductor, while along the zigzag direction a semiconductor-to-metal transition occurs beyond –8%. Additional *ab initio* calculations based on many-body perturbation theory confirm the ability of strained $MoTe_2$ to absorb radiation in the telecom range, thus suggesting the application of this material as a photon absorber at corresponding frequencies upon suitable strain modulation. Equipped with this knowledge, we examine the electronic properties of the vdW HS formed by $MoTe_2$ and WSe_2. This system is subject to intrinsic strain caused by the lattice mismatch between the constituents. In addition to this scenario, we also explore how the electronic and optical of the properties $MoTe_2/WSe_2$ bilayer are modified upon applied biaxial strain up to ±2%. The HS has a type−II level alignment and a direct band gap. Under compressive strain, the optical gap increases, reaching a size compatible with the telecom frequencies, while it reduces upon tensile strain.



[1] Ramzan, M.S. Cocchi, C. Nanomaterials, 13, 2740 (2023).