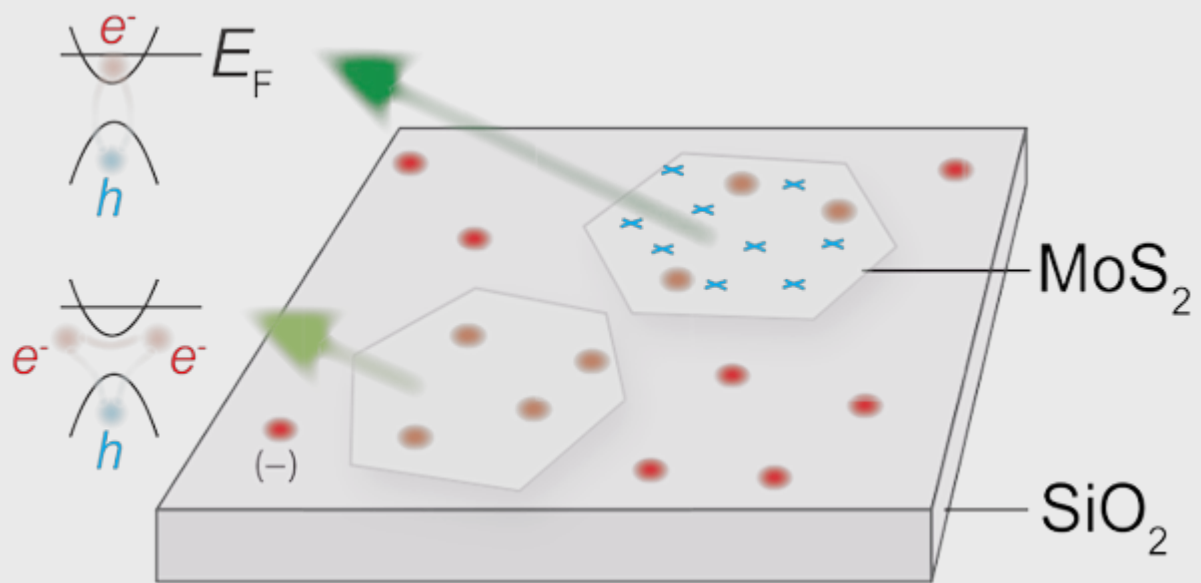


Weakly Trapped, Charged, and Free Excitons in Single-Layer MoS₂ in the Presence of Defects, Strain, and Charged Impurities



Article: published in [ACS Nano](#) by César González, [IFIMAC](#) researcher and member of the Department of Theoretical Condensed Matter Physics.

F

ew- and single-layer MoS₂ host substantial densities of defects. They are thought to influence the doping level, the crystal structure, and the binding of electron–hole pairs. We disentangle the concomitant spectroscopic expression of all three effects and identify to what extent they are intrinsic to the material or extrinsic to it, i.e., related to its local environment. We do so by using different sources of MoS₂ -a natural one and one prepared at high pressure and high temperature- and different substrates bringing varying amounts of charged impurities and by separating the contributions of internal strain and doping in Raman spectra. Photoluminescence unveils various optically active excitonic complexes. We discover a defect-bound state having a low binding energy of 20 meV that does not appear sensitive to strain and doping, unlike charged excitons. Conversely, the defect does not significantly dope or strain MoS₂. Scanning tunneling microscopy and density functional theory simulations point to substitutional atoms, presumably individual nitrogen atoms at the sulfur site. Our work shows the way to a systematic understanding of the effect of external and internal fields on the optical properties of two-dimensional materials. [[Full article](#)]