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**Spin Effects in isolated mono- and bilayer molybdenum disulfide Nanowires**[1] LUCAS FERNÁNDEZ SEIVANE[2], XÓCHITL LÓPEZ-LOZANO, University of Texas at San Antonio — Inspired by the recent synthesis of needle-like $MoS_2$ nanoparticles, we have investigated the properties of isolated quasi-one dimensional $MoS_2$ nanowires. These nanostructures deserve a special interest since they constitute one of the smallest self-supported $MoS_2$ systems with promising catalytic properties. A complete description of the edge, electronic and spin properties for different sulfur saturations is extremely important for the future developments of novel $MoS_2$-based nanocatalysts. In this work we have performed ab initio simulations within the Density Functional Theory framework with the SIESTA code to study the structural, electronic and spin properties of quasi-one dimensional $MoS_2$ Nanostructures. We observed that a change in the number of Mo atoms on the unit cell affects greatly the electronic properties. Interestingly, metallic states are found in all the low-energy models. Also, both for mono- and bilayer the spin states are also localized at the active nanowire edges. We also noticed the presence of a variety of spin regimes suggesting the connection between magnetism and its catalytic properties. In spite of the observed pairing of S dimers at the Mo-edge in some cases, we do not observe a Peierls-like metal-insulator transition.

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[2]previous address: Centro Mixto de Investigación en Nanomateriales y Nanotecnología (CSIC—Universidad de Oviedo—Principado de Asturias)

Lucas Fernández Seivane
University of Texas at San Antonio

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