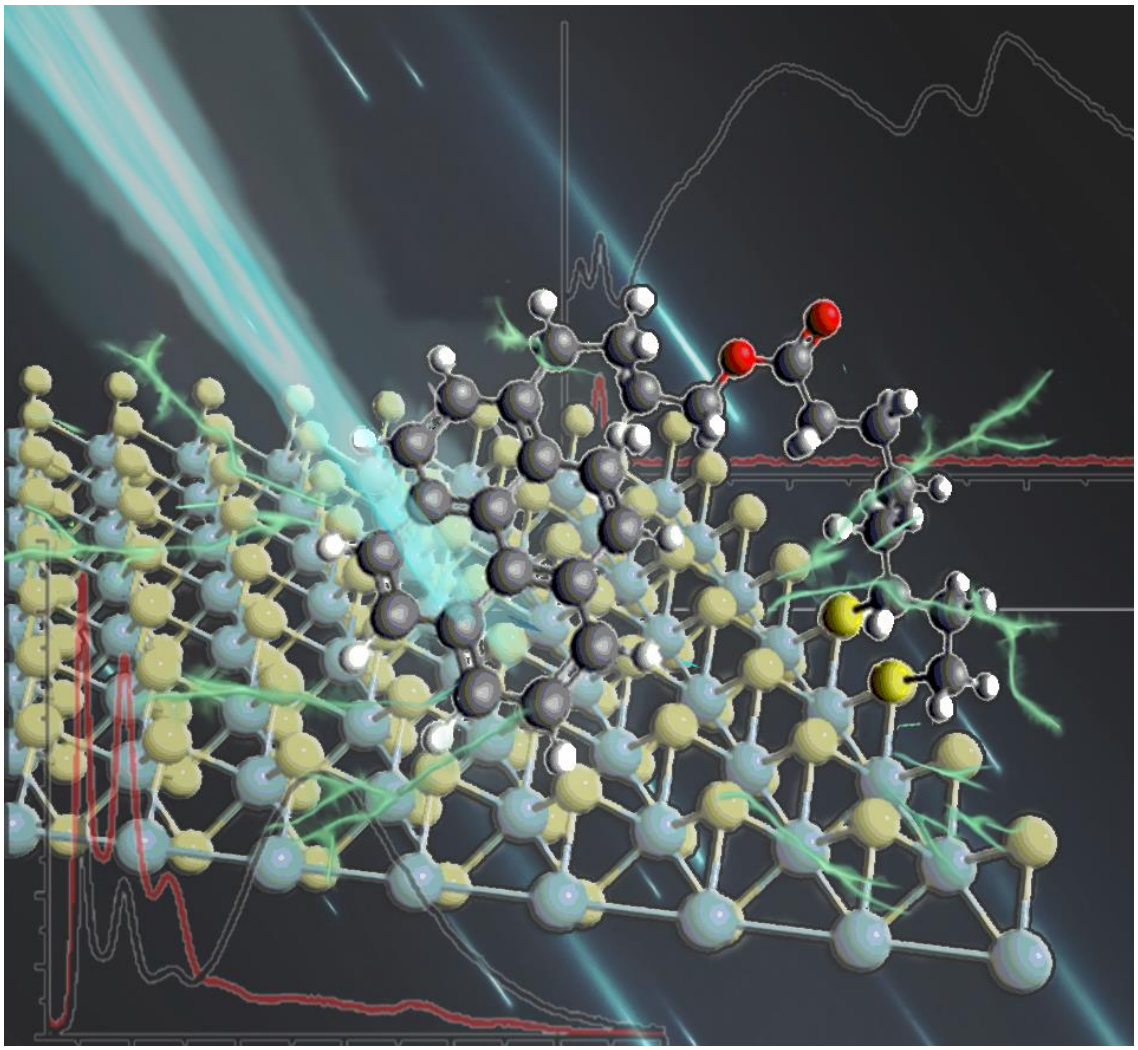
Press Release
Chemical tuning MoS2 for energy applications: Living on the edge

Layered transition metal dichalcogenides, represented by MoS_2, that could chemically couple with organic addends might easily realize their enormous potential for optoelectronics and materials. However, MoS_2 tends to be rather inert – chalcogen atoms in the basal plane are saturated and not highly reactive, while the metal atoms are embedded beneath the chalcogen layer and thus are not susceptible to functionalization. A new interdisciplinary study from groups at the Theoretical and Physical Chemistry Institute (TPCI) of the National Hellenic Research Foundation (NHRF), Athens, the Institut des Materiaux Jean Rouxel – CNRS Nantes, France, the Instituto de Nanociencia, Universidad de Zaragoza, Spain, all within the H2020 Marie Curie ITN "Enabling Excellence" project, and Chimie des Interactions Plasma-Surface, University of Mons, Belgium, proves that 1,2-dithiolane derivatives can covalently anchored preferentially at the MoS_2 sheet edges. This key result presents an important piece to the puzzle of 2D materials' chemistry. "We have recently shown an effective way to exfoliate MoS_2 from the bulk material, while retaining the novel semiconducting properties", says Nikos Tagmatarchis, corresponding author of the study in Athens, "and this unique functionalization strategy allows the realization of a plethora of inorganic-organic hybrid materials incorporating diverse photo- and electro-active moieties en route to the development of sustainable energy conversion schemes".

MoS_2 can be chemically functionalized with organic functional units, to develop innovative hybrid materials suitable for energy conversion. Collaborative efforts between experimental and modelling teams at the Theoretical and Physical Chemistry Institute – National Hellenic Research Foundation, Greece, and the Institut des Materiaux Jean Rouxel – CNRS Nantes, France, respectively, reveal that chemical functionalization occurs preferentially on MoS_2 edge sites and can also be viewed as filling vacant sulfur edge sites. "When photoactive components are attached to MoS_2 edges, visible light illumination promotes efficient charge-transfer within the hybrid material" says Nikos Tagmatarchis and highlights "research along those lines may result in the construction of innovative solar and photoelectrochemical cells with high efficiencies".



Article Reference:

"Functionalization of MoS_2 with 1,2-dithiolanes: toward donor-acceptor nanohybrids for energy conversion"

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