

### البحث الثالث (بحث رقم 6 في قائمة الأبحاث محل تقييم اللجنة الموقرة )

<b>Title</b>	Trigonal antiprismatic Co(II) single molecule magnets with large uniaxial anisotropies: importance of Raman and tunneling mechanisms
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#### **Abstract:**

MoS<sub>2</sub> is a very attractive material and has been well studied for potential applications in various areas. However, due to the wide variety of factors affecting the molecular and electronic structure of MoS<sub>2</sub>, several contradictory reports about the adsorptive and photocatalytic properties of such materials have been published. In most of these reports, the effect of the actual phase of the materials on the properties was neglected. Here, different phases of MoS<sub>2</sub> nanosheets (1T/2H, 1T/3R and 2H) have been obtained using the hydrothermal method with different Mo : S molar ratios and different autoclave filling ratios. The obtained materials have been thoroughly characterized using Raman, UV-vis, powder XRD, SEM, TEM and XPS measurements in order to accurately identify the existing phases in each material. A comparative study of the photocatalytic organic dye degradation efficiency under white light irradiation has been conducted using methyl orange to correlate the different activity of each material to their respective phase composition. The results indicate a much higher performance of the 1T/2H phase compared to

the 2H and 3R phases. Detailed computational studies of the different phases revealed the emergence of mid-gap states upon introducing 1T sites into the 2H lattice. This leads to the improvement of the photocatalytic activity of 1T/2H compared to the other prepared materials.