**Supplementary Information (only for review):**

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**Fig. S1**: Raman spectra collected from MoS2 bulk and MoS2 nanocrystals. We noticed a slight peak shift toward right side MoS2 nanocrystals in comparison to bulk crystal.





**Fig. S2**: Core-level spectra of Mo3d and S2p region from MoS2 bulk. Open circles represent the experimental data and the solid lines are curve-fitted deconvolution peaks after Shirley background subtraction. Core-level spectra of Mo3d region has a predominant spin-orbit doublet (Mo3d5/2 and Mo3d3/2, Δ=3.13 eV) along with corresponding S2p region spin-orbit doublet (Δ=1.18 eV). A minor peak (Mo3d3/2) at higher binding energy is associated with the Mo(VI) oxidation state resulting from surface oxidation.





**Fig S3**: Core-level spectra of Mo3d and S2p region from MoS2 nanocrystals. Open circles represent the experimental data and the solid lines are curve-fitted deconvolution peaks after Shirley background subtraction. Core-level spectra of Mo3d region has a predominant spin-orbit doublet (Mo3d5/2 and Mo3d3/2, Δ=3.13 eV) along with corresponding S2p region spin-orbit doublet (Δ=1.18 eV). A secondary Mo3d doublet peak with a corresponding S2p doublet on the higher binding energy is associated with MoS3 phase. And a third Mo3d peak at higher binding energy with an associated O1s peak is associated with the Mo(VI)O3.



**Fig. S4**: ESR spectra measured from bulk MoS2 bulk crystal. This spectra shows unwanted Re and Fe impurities along with sulfur vacancies (intrinsic).



**Fig. S5**: ESR spectra measured on Mo precursor. We verified that the broad background signal comes from the cavity background. The sharp signal is the result of random spike, not due to the sample.



**Fig. S6**: ESR spectra measured on S source, which shows weak paramagnetic impurities present in the precursor.



**Fig. S7**: ESR spectra measured on Ar-annealed MoS2 nanocrystals measured at 25 K (in black) and 40 K (in green). The spectra remain practically unchanged as a function of temperature.