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First-principles study of Raman active modes in MoS_2 intercalated with Ag

Two-dimensional layered materials have been subject of increased research interest ever since a single layer of graphen has been obtained by mechanical exfoliation in 2004 [1]. In particular, the transition metal dichalcogenides (TMDs) with the general formula MX_2, where M is a transition metal (Mo, W) and X a chalcogen atom (S, Se, Te), have already shown a wide range of technologically relevant properties when scaled down from bulk to few-layer systems. For example, bulk MoS_2 has an indirect band gap of 1.29 eV, which becomes a direct band gap of 1.8 eV when a single layer of MoS_2 is considered [2].

Precise characterization of two-dimensional materials is crucial for exact control of their properties that vary with the number of layers. Raman spectroscopy has become the key experimental technique in this sense, due to its nondestructive nature and the ability to identify even small structural and electronic changes.

Here, we present a combined experimental and theoretical study of the Raman active modes of few-layer MoS2 intercalated with silver. Using Density Functional Theory (DFT) we predict a significant red shift of all Raman active modes of MoS_2 upon Ag intercalation and with increasing Ag concentration in few-layer systems (see figure 1 for results in 2L). However, this effect subsides as the number of MoS_2 layers grows as is supported by the linear chain model for the low-frequency shear and breathing modes for systems with the number of layers corresponding to experimental sample thicknesses. While high-frequency intralayer Raman modes have been extensively studied, we specifically focus on low-frequency interlayer Raman modes that are more susceptible to changes of interlayer couplings [3] and are modified due to presence of silver in the van-der-Waals gap of MoS_2.

References

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Figures

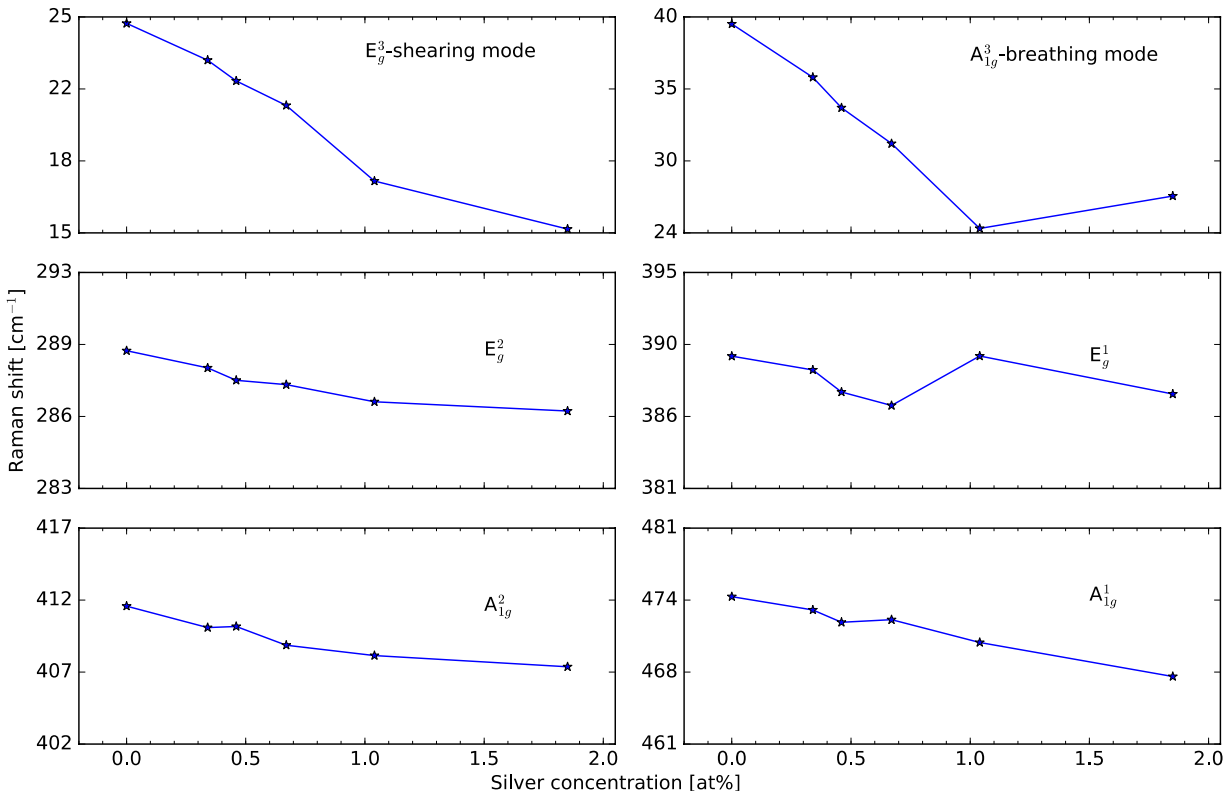

Figure 1: Raman active modes of 2L MoS_2 as a function of silver concentration after intercalation of silver in the van-der-Waals gap of bilayer MoS_2.