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# $Si@MoS_2$ Core-Shell Architecture: Characterizations and Implications for Nanophotonic Applications

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Transition metal dichalcogenides (TMDs) are attractive for next-generation photonics due to their large exciton binding energy and exciton transition dipole moment. However, the atomically thin nature of TMDs yields limited absorption and emission of the incoming electromagnetic (EM) field. This makes isolated TMDs inappropriate for use in optical-to-electrical conversion applications. Recently, TMD-encapsulated nanoparticles have presented a potential avenue for strong light-matter interactions by leveraging the functionality of the core material[1,2,3]. This geometry has potential applications in nanophotonic devices such as all-optical switches, exciton−polariton lasers, and quantum information processing, as well as various optoelectronic applications such as ultrasensitive sensing, light-emitting devices, and solar cells[1].

In order to improve the functionality of TMDs, previous reports have encapsulated plasmonic nanoparticles with TMDs and confined the EM field to the gap between the nanoparticle and the semiconductor to enhance photoluminescence (PL) at the nanoscale[4]. Such core-shell structures maximize the interaction area between the TMD and the core, improving energy coupling and light-matter interaction. Recent work hybridizing high refractive index dielectric nanoparticles with quantum emitters has shown unusual and attractive functionality, such as directional scattering[1]. Harnessing these constituents in a core-shell architecture could result in reduced losses and enhanced resonance of electric and magnetic near fields[5]. The coupling of Mie magnetic dipole mode of the nanoparticle and exciton transitions in the semiconductor may also enable longer exciton lifetimes[5]. Therefore, improved energy transfer and enhanced absorption could be realized.

Here, we demonstrate the first experimentally synthesized $Si@MoS_2$ architecture and utilize spectroscopic information obtained through transmission electron microscopy (TEM) and scanning TEM (STEM) techniques, such as electron energy loss spectroscopy (EELS), to conduct microanalysis. In our architecture, we use silicon polycrystalline nanoparticles (n = 3.5) of radii ranging predominantly between 70 and 120 nm as the spherical core structure. We encapsulate the nanoparticles on rigid substrates with chemical vapor deposition (CVD)-grown $MoS_2$, where the shell thickness is predominantly between 5 to 15 layers. We observe the complete and conformal encapsulation through TEM imaging of isolated $Si@MoS_2$ structures (**Figure 1**). The $MoS_2$ shell layers are clearly visible in **Figure 1B** with total thickness of 4.38 nm corresponding to approximately 7 layers. The architecture observed via TEM was further supported by Raman spectroscopy.

We then confirm the elemental composition of the shell through energy dispersive x-ray spectroscopy (EDS). We further note the absence of silicon core oxidation through core-loss EELS[6], and identify the expected characteristic low-loss peaks for silicon at ~17 eV[7] and ~34 eV[8] and $MoS_2$ at ~22 eV[9] as shown in **Figure 2**. We use the least-square function to fit Lorentz curves to these known characteristic peaks and derive the chemical composition map in **Figure 2B**. The map validates the architecture observed through TEM imaging in **Figure 1**.

The successful demonstration of $Si@MoS_2$ at this length scale offers an experimental assessment of the potential of TMD/high-index dielectric hybrid systems in this unique geometry[1,2]. From here, we aim to follow with optical measurements to observe the coupling between the two materials and other exotic optical phenomena in this unique architecture. This research stands as a starting point to multiple avenues for future microanalysis research that can optimize the optical response of the core-shell heterostructure. For example, exploring the effect of core diameter

or shell thickness, measuring response from particle clusters rather than isolated particles, and encapsulating with different two dimensional materials such as multiferroic layered systems, are some approaches.

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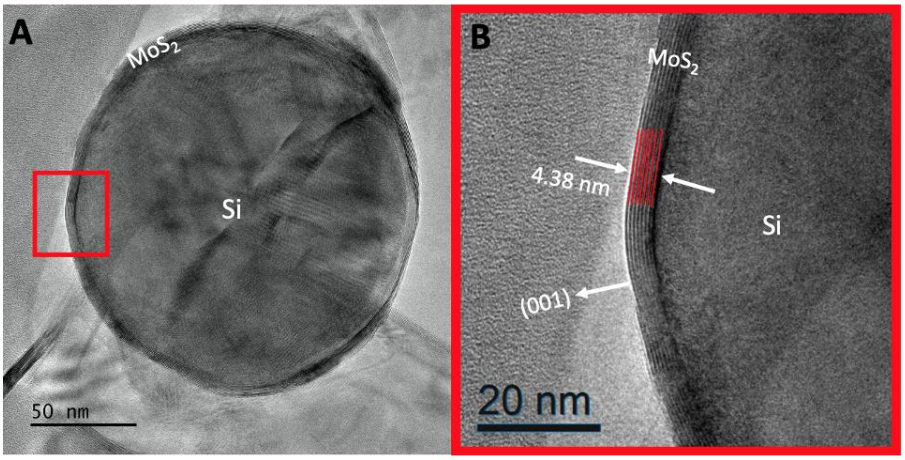


**Figure 1.** TEM image of an isolated Si@MoS2 on lacey carbon copper TEM grid. A) Silicon polycrystalline core of diameter ~150 nm is encapsulated with shell layers of CVD-grown MoS2. B) Magnified image of region outlined in (A) showing the (001) atomic planes of MoS2 outlined with red lines. Seven MoS2 layers are outlined for clarity.

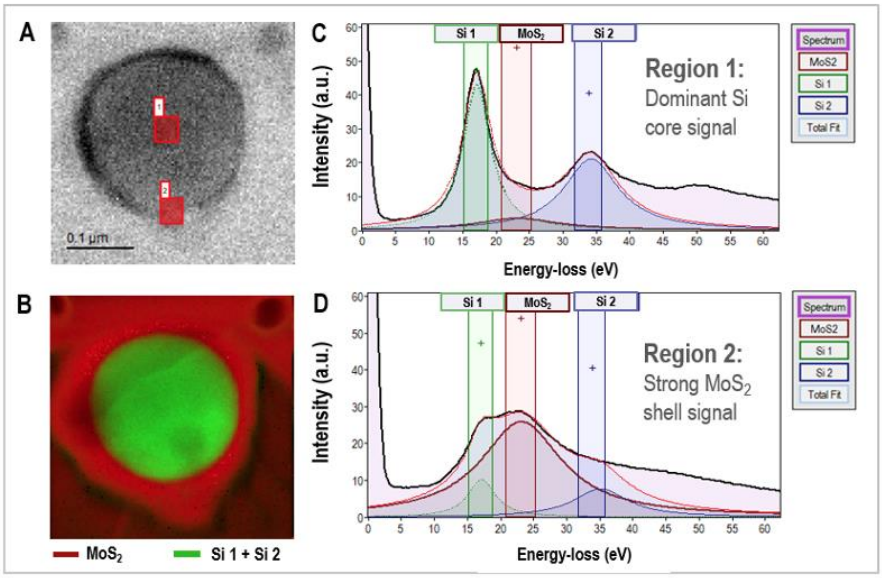


**Figure 2.** EELS of the Si@MoS2 heterostructure. A) STEM image of Si@MoS2, with two EELS regions of interest outlined in red. B) Chemical composition map resulting from EELS spectra showing the green silicon core and strong red MoS2 shell. C) Region 1 from (A) is dominated by the silicon core peaks at ~17 eV and ~34 eV. D) Region 2 from (A) is dominated by a mix of silicon core peaks and a strong MoS2 shell peak at ~22 eV.

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