Lithium sulfur batteries (LSBs) have been regarded as the most promising energy storage system for the next generation that draws tremendous attention over decades owing to their high energy density based on the multi-electron chemical reaction far beyond the conventional lithium ion batteries. In addition to the naturally abundance, cheapness, non-toxicity and environmental friendliness of elemental sulfur, LSBs becomes particular attractive for the future development of vehicle electrification, grid scale application of the renewables and more advanced portable electronic devices. Despite of these advantages, insulating nature of elemental sulfur and lithium sulfide, over 80% of volume change between the conversions of sulfur and lithium sulfide and “shuttle effect” induced by the highly dissolvable nature of long-chain lithium polysulfide into the electrolyte remains as the major obstacle for the practical application of LSBs.

While transition metal oxides and sulfides were recently demonstrated that have strong affinity to the polysulfides. However, their intrinsic semi-conductive properties limit their further utilization. Herein, we proposed a new type of anchoring material, transition metal selenides which is not only more conductive but also capable of effective confinement of lithium polysulfides. By chemical vapor deposition (CVD) method, triangular shaped molybdenum diselenide (MoSe$_2$) nanoflakes with less than 10 layers stacking were successfully synthesized and uniformly distributed on the nitrogen doped graphene. We found that our material enables the better electrochemical performance with faster redox kinetics and more stable cycling. MoSe$_2$/N-rGO/S delivered the initial discharge capacity of 1309 mAh/g and 1028 mAh/g at 0.05 C and 0.2 C, respectively with 86.3% of cycling retention and 98% Coulombic efficiency. Combining the studies of density functional theory (DFT) simulation, adsorption test, X-ray photoelectron spectroscopy (XPS) analysis and Transmission electron microscopy (TEM) technique, we discovered that the selenium edges of MoSe$_2$ possess strong binding energy to lithium polysulfides, while the lithium ion diffusion barrier on the surface of MoSe$_2$ is lower in the comparison of graphene surface. The reported finding provides a positive insight into the role of transition mental selenides that could be an alternative anchoring material for the cathode material design.