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Phase-Engineered Heterostructures of Mo2C via Plasma-Assisted Selenization and Sulfurization Processes for Plasmon-Free Surface-Enhanced Raman Spectroscopy and Excellent Hydrogen Evolution Reaction

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Abstract:

Two-dimensional (2D) materials such as transition metal carbides (TMCs) and dichalcogenides (TMDs) have shown great potential in surface-enhanced Raman spectroscopy (SERS) and electrocatalytic hydrogen evaluation reaction (HER) applications due to their unique electronic properties and tunable phases. In this work, we fabricated Mo2C using the chemical vapor deposition (CVD) method and then transformed it into Mo2C/MoOx, Mo2C/MoS2, and Mo2C/MoSe2 heterostructures through thermal oxidation, plasma-assisted sulfurization, and selenization, respectively. The phase engineering of the MoS2 and MoSe2 layers to 1T and 2H-rich phases was achieved at 350 and 550 0C, respectively, which gave a way toward tuning their electronic properties. The 1T-rich Mo2C/MoS2 heterostructure exhibited superior SERS sensitivity, detecting rhodamine B (RhB) at concentrations as low as 10-10 M, attributed to the high density of states and "hot spots" that enhance charge transfer and local electromagnetic fields. Furthermore, Mo2C/MoSe2 showed a detection limit of 10-9 M, while 2H-rich phases had slightly reduced sensitivity owing to their semiconducting nature. Heterostructures indeed showed parallel performance in HER, whereby the structure of Mo2C/MoSe2 treated at 350 0C exhibited an improved Tafel slope of 66 mV/dec, with overpotential of 257 mV at 10 mA/cm2. Under similar conditions, Mo2C/MoS2 demonstrated enhanced catalytic activity and stability over longer operation. This study provides insights into the development of phase-engineered Mo2C-based heterostructures, highlighting their potential as highly sensitive SERS substrates and efficient HER catalysts and opens new strategies to fabricate high-quality TMCs and TMDs heterostructures with metal-semiconductor interface.

Key words: Mo2C, Heterostructures, Phase engineering, SERS, HER

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