Comprehensive Study of Interface Chemistry and Electrical Property of Metal Contacts on TMDs

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Transition metal dichalcogenides (TMDs) have been introduced due to their exceptional electronic, optical mechanical, and magnetic properties, even in atomically thin thickness, for advanced electronic, optoelectronic, and spintronic devices [1]. However, the limitations in tuning the Schottky barrier height with metal contacts, based on work function greatly hinder efficient carrier injection and electronic performance of TMD-based devices [2]. This study examines contact interfaces and their relationship to electrical contact characteristics. The research encompasses interface chemistry, band alignment, and electronic contact properties of Ni, Ag, Bi, Co and Sn.

An ultrahigh vacuum (UHV) cluster system was employed to investigate the contact properties where in-situ X-ray Photoelectron Spectroscopy (XPS) showed the contact bonding features of metal/TMD interfaces. Ni and Co contacts exhibited stronger bonds with TMD surfaces, resembling covalent-like interfaces, with notable interface reaction products resulting from annealing. However, Bi and Sn showed no robust chemical bonding features under the XPS analysis and van der Waals contact interface was formed due to a weak interaction between metal and TMD. The subsequent ex-situ atomic force microscopy (AFM) measurement supported these contact interface properties. The subsequent electrical characterization using XPS and scanning tunneling microscopy (STM) suggests that the roles of surface defect impact the metal contacts as well. In conclusion, comprehensive research and investigation of metal materials and their contact interface properties with TMDs have shed light on the potential and advantages of metal contact studies.

v; van der Waals bonding interface **n; n-type friendly** **☑; Investigated**
c; covalent bonding interface **p; p-type friendly**

	MoS_2			$MoSe_2$			$MoTe_2$			WS_2			WSe_2			WTe_2		
Ag	☑	v	n	☑	v	n	☑	v	n	☑	v	n	☑	v	n	☑	v	
Ni	☑	c		☑	c		☑	c		☑	c		☑	c	p	☑	c	
Bi	☑	v	n	☑	v	n	☑	v	n	☑	v	n	☑	v	n			
Co	☑	c	p							☑	c	p	☑	c	p			
Sn	☑	v	n	☑	v	n				☑	v	n	☑	v	n			

Table 1. Summary of contact interface investigations.

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