Designing Metal and Semiconductor Contact Heterostructures to Two-Dimensional $MoSi_2N_4$ and WSi_2N_4

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The recent discovery of two-dimensional (2D) MA_2Z_4 monolayers unravels an exciting material platform for a plethora of device applications [1]. Here we study the heterostructures of MA_2Z_4 using density functional theory (DFT) simulations [2-5]. Focusing on $MoSi_2N_4$ and WSi_2N_4, we investigated three major classes of contacts: (i) 3D metals [2]; (ii) 2D metals [3]; and (3) 2D semiconductors [4,5]. For 3D metal contacts, we found that MoSi2N4 and WSi2N4 exhibit strongly suppressed Fermi level pinning effect [Figure 1(a)]. Intriguingly, the presence of an outer Si-N layer offers a *built-in* protective mechanism that preserves the transport states situating in the inner core layer, thus significantly suppressing interfacial tunnelling barrier and avoiding severe metallization of the VBM and CBM states. For 2D metal contacts, nearly Ohmic and electric-field tunable contacts can be obtained using graphene and NbS_2 [3]. We further perform a comprehensive cataloguing of 2D/2D van der Waals heterostructures (vdWHs) between MA_2Z_4 and other 2D semiconductors [4,5]. By simulating 52 different types of MA_2Z_4 vdWHs, several candidate structures with excellent solar cell conversion efficiency reaching well over 20% are identified. Furthermore, we found that $MoSi_2N_4$-and WSi_2N_4-based vdWHs typically exhibit strong optical absorption in the ultraviolet (UV) regime, suggesting their potential for UV photonics applications [Figure 1(b)]. Our findings uncover the contact properties of $MoSi_2N_4$ and WSi_2N_4 and reveal the opportunities of MA_2Z_4 as an emerging 2D material family towards the realization of novel solid-state technology beyond the silicon era.

References

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Figures

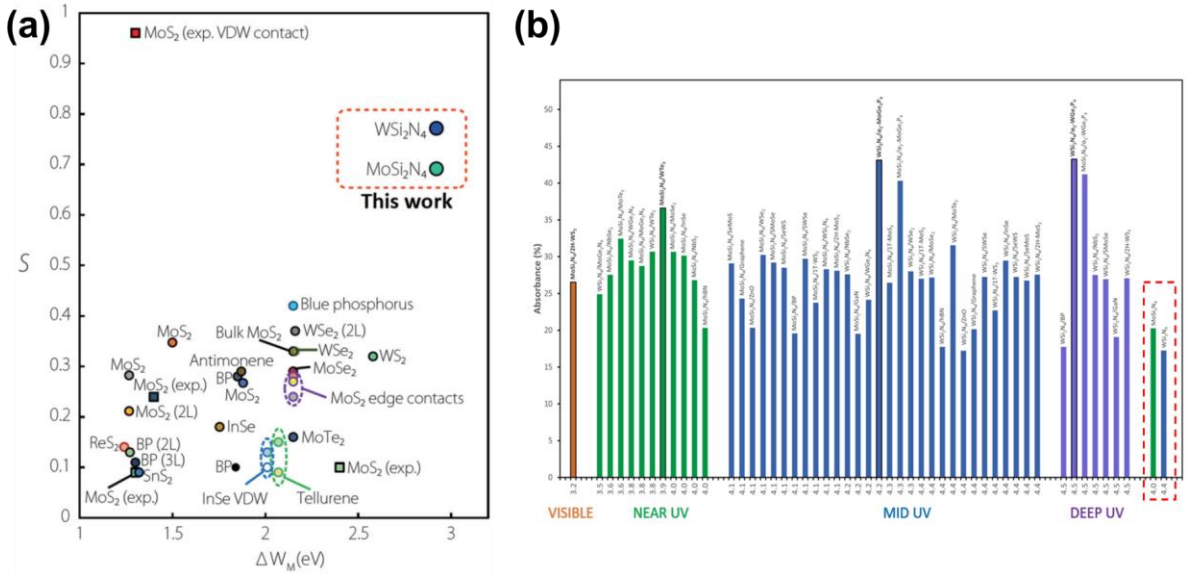

Figure 1: (a) Strongly suppressed FLP effect in $MoSi_2N_4$ and WSi_2N_4 metal contacts [2]. (b) 2D/2D VDWHs based on $MoSi_2N_4$ and WSi_2N_4 exhibit strong optical absorption in the UV regime [5].