Cataloguing $MoSi_2N_4$ and WSi_2N_4 van der Waals Heterostructures: An Exceptional Material Platform for Excitonic Solar Cell Applications

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Two-dimensional (2D) materials van der Waals heterostructures (vdWHs) provides a revolutionary route towards high-performance solar energy conversion devices beyond the conventional silicon-based *pn* junction solar cells.[1,2] Despite tremendous research progress accomplished in recent years, the searches of vdWHs with exceptional excitonic solar cell conversion efficiency and optical properties remain an open theoretical and experimental quest.[3,4] Here we show that the vdWH family composed of $MoSi_2N_4$ and WSi_2N_4 monolayers provides a compelling material platform for developing high-performance ultrathin excitonic solar cells and photonics devices. Using first-principle calculations, we construct and classify 51 types of $MoSi_2N_4$ and WSi_2N_4-based [(Mo,W)Si_2N_4] vdWHs composed of various metallic, semimetallic, semiconducting, insulating and topological 2D materials. Intriguingly, $MoSi_2N_4$/(InSe, WSe_2) are identified as Type-II vdWHs with exceptional excitonic solar cell power conversion efficiency reaching well over 20%, which are competitive to state-of-art silicon solar cells. The (Mo,W)Si_2N_4 vdWH family exhibits strong optical absorption in both the visible and UV regimes. Exceedingly large peak UV absorptions over 40%, approaching the maximum absorption limit of a free-standing 2D material, can be achieved in (Mo,W)Si_2N_4/α_2-(Mo,W)Ge_2P_4 vdWHs. Our findings unravel the enormous potential of (Mo,W)Si_2N_4 vdWHs in designing ultimately compact excitonic solar cell device technology.

References

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Figures

Figure 1: (Mo,W)Si_2N_4-based vdWHs as promising candidates for high efficiency excitonic solar cells