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Supporting Information

Nature of novel hBP-XMY (M=Mo, W; (X≠Y)=S, Se, Te) van der Waals heterostructures for optoelectronic and photocatalytic applications

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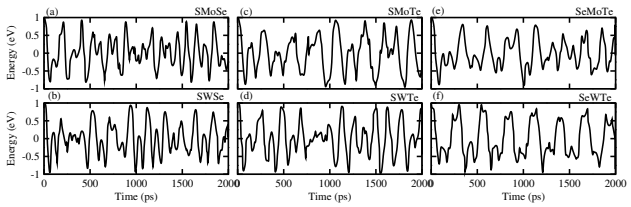

Fig.S 1: Thermal stabilities of strained hBP and XMY (M=Mo, W; (X≠Y)=S,Se,Te) monolayers

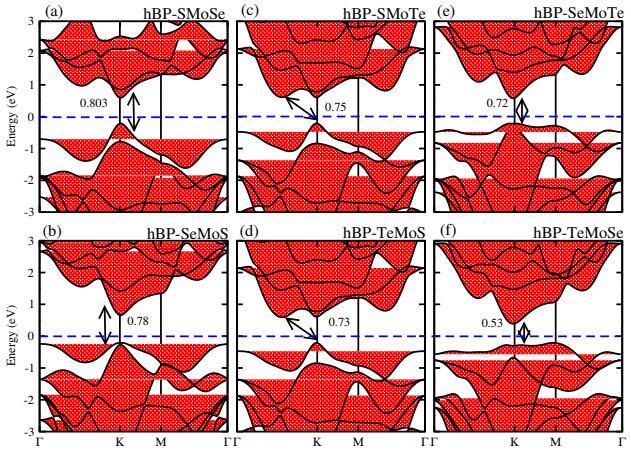

Fig.S 2: Electronic band structure of hBP-XMY (M=Mo; (X≠Y)=S, Se, Te) vdW heterostructures for model-I((a)-(e)) and model-II ((b)-(f)) using PBE calculation

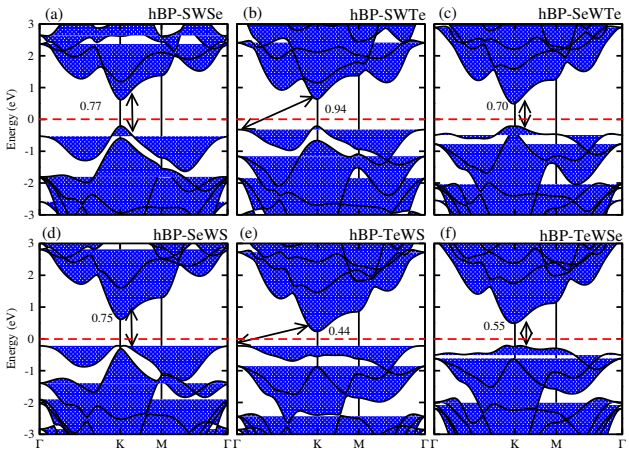

Fig.S 3: Electronic band structure of hBP-XMY (M=W; (X≠Y)=S, Se, Te) vdW heterostructures for model-I((a)-(e)) and model-II ((b)-(f)) using PBE calculation

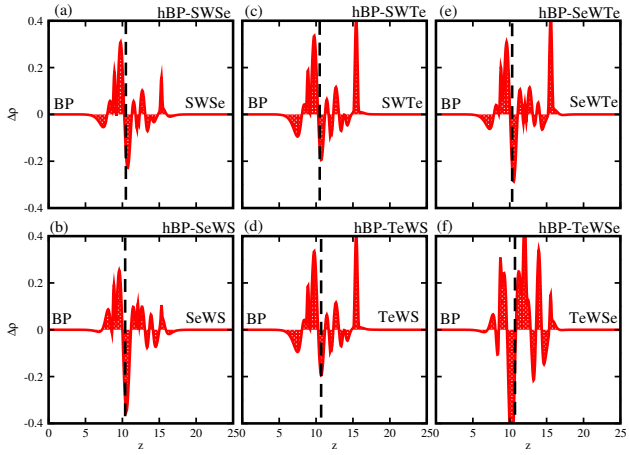

Fig.S 4: Planer-averaged charge density difference of hBP-XMY (M= W; (X≠Y)=S, Se, Te) vdW heterostructures for model-I((a)-(e)) and model-II ((b)-(f))

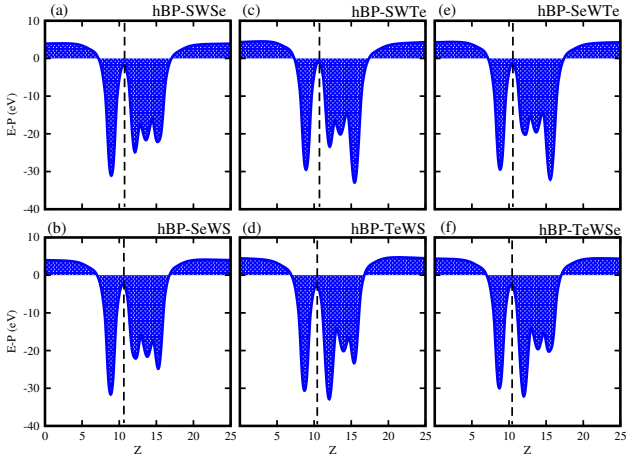

Fig.S 5: Plane-averaged charge density difference of hBP-XMY (M= W; (X≠Y)=S, Se, Te) vdW heterostructures for model-I((a)-(e)) and model-II ((b)-(f))