First principles study on monolayer GeTe as an anode material for multivalent ion batteries

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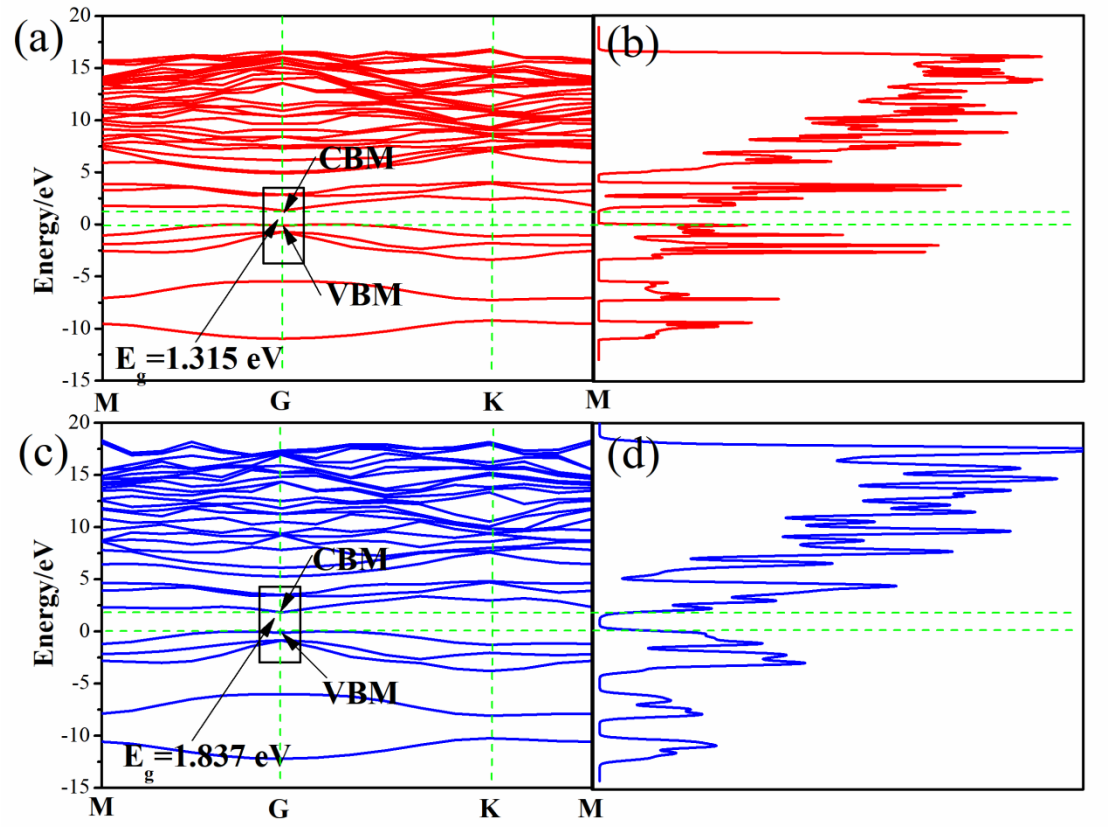

Fig. S1 Band structure and corresponding density of states of monolayer GeTe with (a-b) GGA-PBE and (c-d) HSE06 function

Table S1

Comparison of volume expansion values between some common two-dimensional materials and monolayer GeTe in different metal ion batteries

	Li	Na	K	Al	Mg	Ca
	volume expansion %	volume expansion %	volume expansion %	volume expansion %	volume expansion %	volume expansion %
GeTe (this work)				14.3	15.7	25.8
Ge[1]	253	207	351		231	389
BGe[2]					5.63	
a-C_3N_2[3]	4					
Phosphoene[4]		16				
MoS_2[5]		27				
graphite[6]		12				
Red phosphorus[7]		491				
BSi[8]	33					
Si[9]	300					
SiOx[10]	150					
Si/Graphite[11]	74.4					
Sn[12]	260					
$GeSe_2$[13]	200					

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