Supporting information

Re-examining the Chevrel phase Mo_6S_8 cathode for Mg intercalation from an electronic structure perspective

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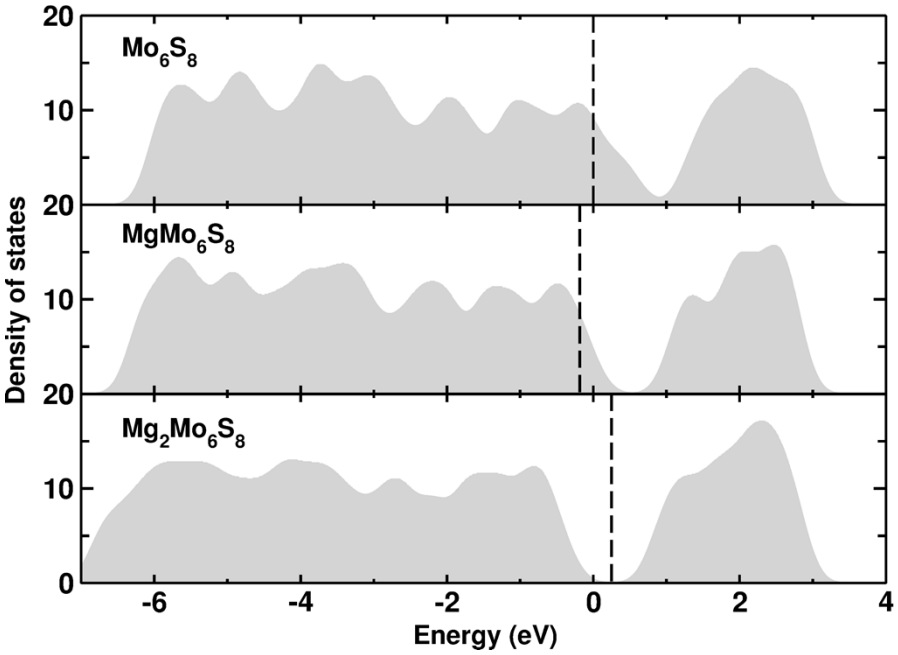
Table S1: A comparison of the calculated lattice parameters for Mo_6S_8, $MgMo_6S_8$, and $Mg_2Mo_6S_8$ at U = 0 and U = 3.16 eV.

Structure	Methods	a (Å)	b (Å)	c (Å)	α (°)	β (°)	γ (°)
Mo_6S_8	GGA+U	6.446	-	-	91.50	-	-
	GGA	6.509	-	-	91.59	-	-
$MgMo_6S_8$	GGA+U	6.508	6.514	6.509	92.79	92.79	93.67
	GGA	6.564	6.573	6.565	93.13	93.12	93.93
$Mg_2Mo_6S_8$	GGA+U	6.562	-	-	92.82	-	-
	GGA	6.601	-	-	92.78	-	-

Using standard PBE-GGA functional, the calculated lattice constants are slightly larger than the results obtained with a U correction.

Figure S1: Total electronic density of states for Mo_6S_8, $MgMo_6S_8$ and $Mg_2Mo_6S_8$, simulated using the PBE-GGA functional.



The total densities of states obtained using standard PBE-GGA functional are qualitatively the same as the results at U = 3.16 eV. However, the band gap in $Mg_2Mo_6S_8$ is substantially underestimated because the Mo d-electrons are treated too delocalized in the PBE functional.