

Supplementary Information

Table 1 Moments of $E(0, R_y, R_z)$ for the X-H bond LMO in second row hydrides. The bond LMO under analysis in Case 2 has a bond length of 1.527543 a.u.

System	Case 1			Case 2		
	$\langle R_{yz}^0 \rangle$	$\langle R_z \rangle$	R_z^{\max}	$\langle R_{yz}^0 \rangle$	$\langle R_z \rangle$	R_z^{\max}
NaH	0.448	-1.504	-1.731	0.461	-1.266	-1.401
MgH ₂	0.503	-1.220	-1.436	0.519	-1.142	-1.292
AlH ₃	0.556	-1.028	-1.193	0.562	-1.010	-1.160
SiH ₄	0.610	-0.847	-0.959	0.602	-0.859	-0.978
PH ₃	0.650	-0.653	-0.764	0.628	-0.661	-0.779
SH ₂	0.690	-0.448	-0.586	0.652	-0.413	0.581
ClH	0.739	-0.280	-0.429	0.690	-0.170	0.397