

## Crystal growth, dislocation, thermodynamic and optical properties, electronic structure of Mg<sub>2</sub>SiO<sub>4</sub> single crystal

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**Table S1.** Calculated surface energy of the Mg<sub>2</sub>SiO<sub>4</sub> crystal on (100), (010), and (001)  
faces. (ICSD#062525) <sup>1</sup>

Crystalline surface	Lattice period	Surface energy (eV/Å <sup>2</sup> )	Minimum value (eV/Å <sup>2</sup> )
(100)	0	0.158425932	0.158425932
	0.008	0.218535088	
	0.074	0.277163145	
	0.222	0.243540379	
	0.223	0.167838601	
	0.234	0.168919244	
	0.266	0.16777471	
	0.277	0.24356673	
	0.278	0.277364151	
	0.426	0.218532075	
	0.492	0.15956242	
	0.5	0.159770295	
	0.508	0.2335502	
	0.574	0.277451907	
	0.722	0.243566907	
	0.723	0.167783501	
	0.734	0.169047813	
	0.766	0.168102012	
	0.777	0.24367907	

	0.778	0.277172548	
	0.926	0.218550025	
	0.992	0.158718862	
	1	0.158434231	
	0	0.253849312	
	0.053	0.096363552	
	0.092	0.192731639	
	0.094	0.208589091	
	0.163	0.201488775	
	0.223	0.062025912	
	0.277	0.20193574	
	0.337	0.208562134	
	0.406	0.192604797	
	0.408	0.096349304	
	0.447	0.253906433	
(010)	0.5	0.253826072	0.061996248
	0.553	0.096357563	
	0.592	0.19252851	
	0.594	0.208802361	
	0.663	0.201447647	
	0.723	0.061996248	
	0.777	0.201431299	
	0.837	0.208423731	
	0.906	0.192516133	
	0.908	0.096338057	
	0.947	0.253916437	
	1	0.253860416	
	0	0.136493261	
	0.033	0.163680952	
	0.25	0.163593889	
	0.467	0.136281502	
(001)	0.5	0.136203992	0.136203992
	0.533	0.163466	
	0.75	0.163577937	
	0.967	0.136322654	
	1	0.136418232	

**Table S2.** The Raman active modes of previous results and this work.

Modes	Previous work <sup>2</sup>	Previous work <sup>3</sup>	This work
$A_g$	966	967	966
	856	-	858
	826	-	826
	609	610	610
	546	548	548
	424	426	423
	340	341	342
	329	334	332
	305	307	305
	227	232	229
	183	183	-
$B_{1g}$	976	-	-
	866	-	-
	839	-	-
	632	-	-
	583	585	-
	434	443	436
	418	-	-
	318	-	319
	260	-	-
	224	-	-
192	-	-	
$B_{2g}$	884	882	883
	588	-	590
	441	-	-
	368	-	-
	324	-	-
	244	244	-
	142	171	-
$B_{3g}$	922	920	922
	595	593	-
	412	426	-
	376	414	-
	318	376	-
	272	-	-
	226	-	-

## Notes and references

1. R. Van der Wal, A. Vos and A. Kirfel, *Acta Crystallographica Section B: Structural Science*, 1987, **43**, 132-143.
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3. P. Richet and F. Guyot, *Journal of Geophysical Research*, 1991, **96**, 11805-11816.