

# Archimedean (4,8)-tessellation of haeckelite ultrathin nanosheets composed of boron and aluminum-group V binary materials

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## Electronic Supplementary Information

Table S1: Haeckelite crystal structure data for all materials presented within the main text. All lattice constants are given in angstrom, Å.  $\alpha$ ,  $\beta$ , and  $\gamma$  refer to crystal cell angles (degrees) of bulk haeckelite crystals.

Material	a	b	c	$\theta_1$	$\theta_2$	$\theta_3$	$\theta_4$	$\alpha$	$\beta$	$\gamma$
H- $B_8N_8$	5.013	5.013	4.229	—	—	—	—	90.00	90.00	90.00
H- $B_8P_8$	6.303	6.303	5.322	—	—	—	—	90.00	90.00	90.00
H- $B_8As_8$	6.689	6.689	5.625	—	—	—	—	90.00	90.00	90.00
H- $B_8Sb_8$	7.352	7.352	6.150	—	—	—	—	90.00	90.00	90.00
H- $B_4N_4$	4.938	4.938	—	95.74	84.26	132.13	134.87	—	—	—
H- $B_4P_4$	6.350	6.350	—	89.53	90.47	135.24	134.77	—	—	—
H- $B_4As_4$	6.707	6.707	—	91.51	88.49	134.25	135.76	—	—	—
H <sub>B</sub> - $B_4As_4$	5.784	5.784	—	102.94	63.52	127.54	109.11	—	—	—
H- $B_4Sb_4$	7.398	7.398	—	92.57	87.43	133.71	136.29	—	—	—
H <sub>B</sub> - $B_4Sb_4$	6.264	6.264	—	102.36	49.81	125.53	110.31	—	—	—
H- $Al_8N_8$	6.167	6.167	5.006	—	—	—	—	90.00	90.00	90.00
H- $Al_8P_4$	7.649	7.648	6.375	—	—	—	—	90.00	90.00	90.00
H- $Al_8As_8$	7.961	7.960	6.646	—	—	—	—	90.00	90.00	90.00
H- $Al_8Sb_8$	6.754	11.099	5.376	—	—	—	—	90.00	90.00	90.00
H- $Al_4N_4$	6.154	6.154	—	93.78	86.22	133.11	136.89	—	—	—
H- $Al_4P_4$	7.749	7.750	—	95.46	85.54	132.27	137.73	—	—	—
H <sub>B</sub> - $Al_4P_4$	6.843	6.844	—	95.08	74.07	130.82	110.63	—	—	—
H- $Al_4As_4$	8.057	8.057	—	95.64	84.36	132.18	137.81	—	—	—
H <sub>B</sub> - $Al_4As_4$	6.925	6.925	—	95.46	71.19	130.30	105.76	—	—	—
H- $Al_4Sb_4$	8.782	8.782	—	95.85	84.15	132.08	137.92	—	—	—
H <sub>B</sub> - $Al_4Sb_4$	7.296	7.295	—	97.48	67.14	129.06	101.87	—	—	—

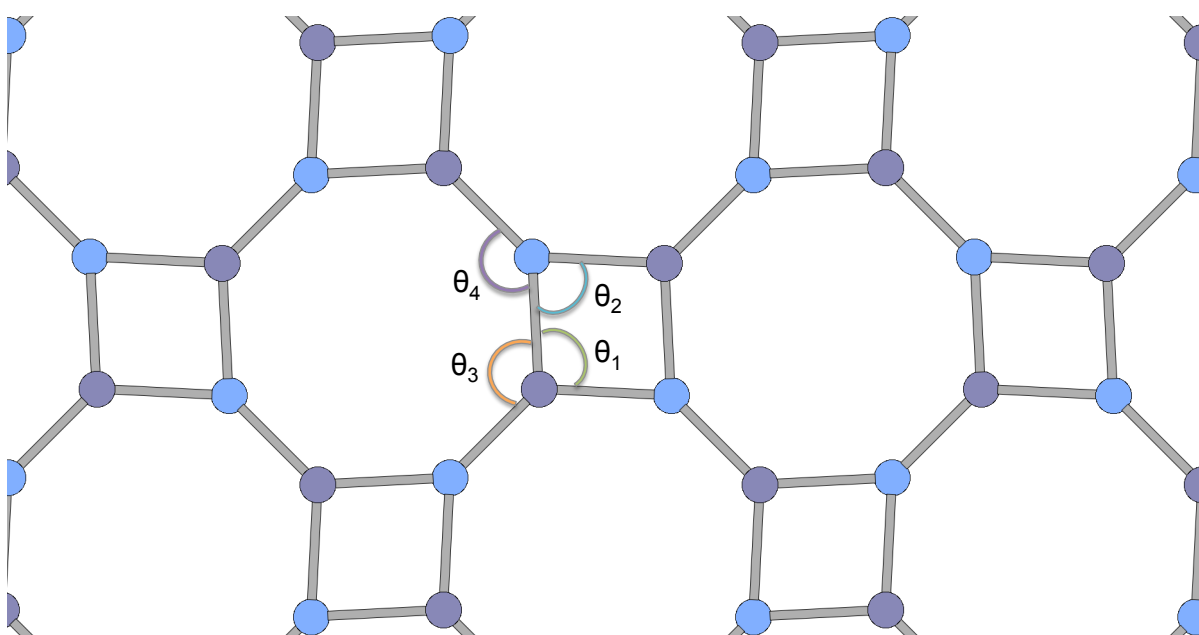


Figure S1: Angles listed in Table S1 for all haeckelite nanosheets and bulk haeckelite crystals.

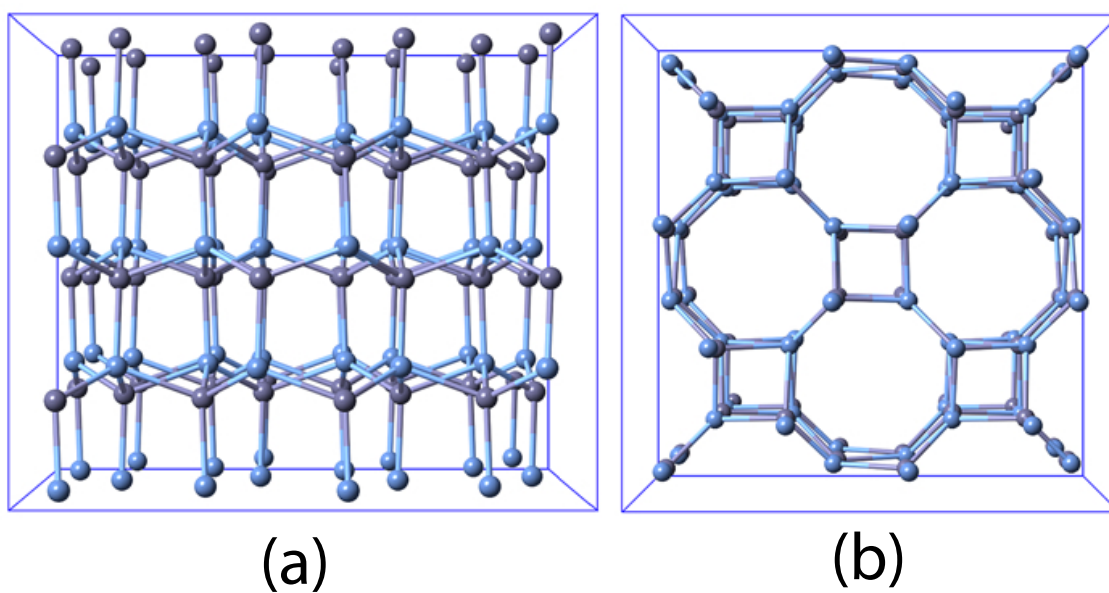


Figure S2: Bulk  $H-B_8N_8$  shown in an expanded  $2 \times 2 \times 2$  cell along (a) (100) and (b) (001) crystallographic directions. This cell is a representative model of all bulk boron and aluminum haeckelite crystals, except for the bulk  $H-Al_8Sb_8$ . Note the color scheme of the elements for all figures in the supplemental is the same as that displayed in the manuscript.

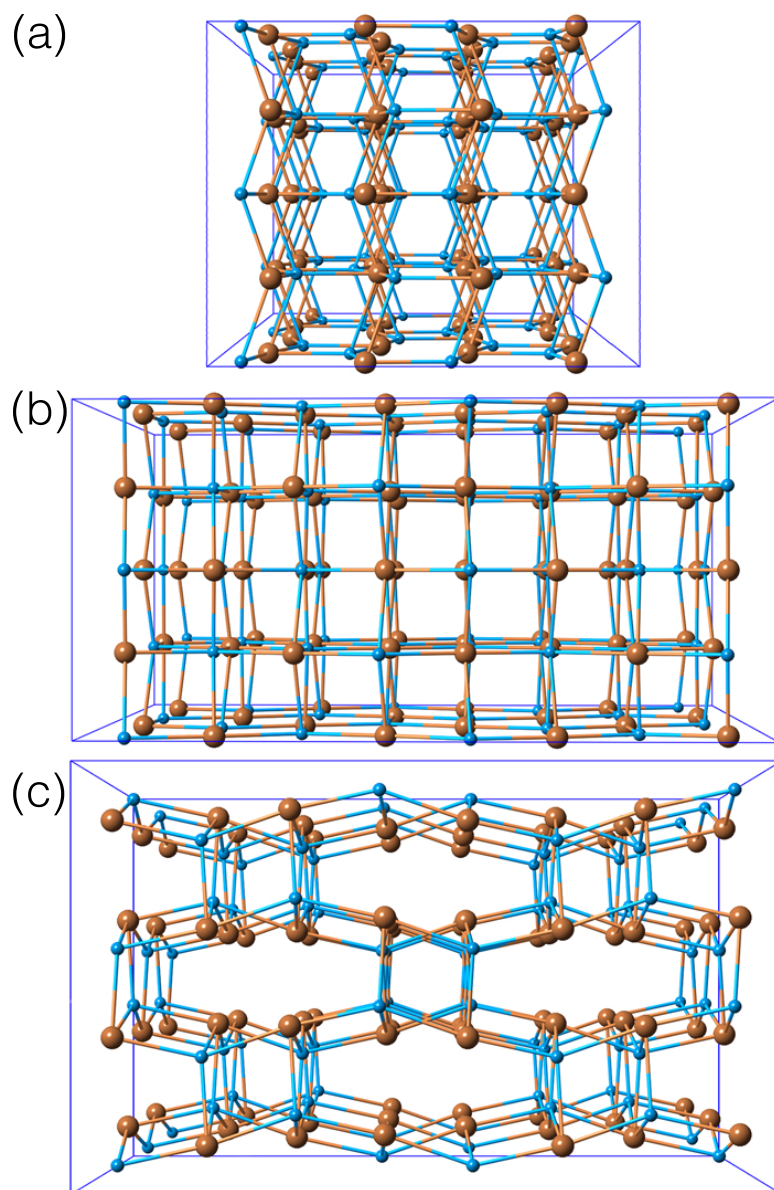


Figure S3: Bulk  $\text{H-Al}_8\text{Sb}_8$  displayed in an expanded  $2 \times 2 \times 2$  cell along (a) (100), (b) (010), and (c) (001) crystallographic directions. We can see in this cell the unique bonding pattern accompanied with five coordinate alumina and antimony elements. Note the color scheme of the elements for all figures in the supplemental is the same as that displayed in the manuscript.