Surface energies of AlN allotropes from first principles:  
Supplemental material

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Structures

In the following tables we list the cell shapes and atom positions used for constructing a  
slab of material for the surface energy calculations.

Table 1: Lattice vectors and fractional coordinates of atoms for the primitive cells used for construction of  
\{100\}, \{110\}, \{111\}, and \{112\} surfaces of the B1 structure. The N-terminated \{111\} slab is obtained by  
exchanging Al and N lattice sites.

|       | \{100\} | \{110\} | \{111\} | \{112\} |
|-------|---------|---------|---------|---------|
| a₁    | 1/2     | -1/2    | 0       | √2/2    | 0       | 0       | 0       | √3/4    | -√6/4   | 0       | √3/2    | 0       | 0       |
| a₂    | 1/2     | 1/2     | 0       | 0       | 0       | 0       | 0       | 0       | 0       | 0       | 0       | √2/2    | 0       |
| a₃    | 0       | 0       | 1       | 0       | 0       | √2/2    | 0       | 0       | 0       | 0       | √3/2    | 0       | √6/2    |
| Al    | 1/2     | 1/2     | 1/2     | 1/2     | 1/2     | 1/2     | 1/2     | 1/6     | 1/6     | 1/6     | 1/6     | 1/6     | 1/6     |
| Al    | 2/3     | 2/3     | 2/3     | 1/3     | 0       | 1/3     | 0       | 1/3     | 0       | 1/3     | 0       | 1/3     | 0       |
| N     | 1/2     | 1/2     | 0       | 0       | 1/2     | 0       | 0       | 1/2     | 0       | 1/2     | 0       | 1/2     | 0       |
| N     | 0       | 0       | 1/2     | 1/2     | 0       | 1/2     | 0       | 1/2     | 0       | 1/2     | 0       | 1/2     | 0       |
| N     | 2/3     | 2/3     | 1/6     | 5/6     | 1/6     | 1/2     | 1/6     | 1/6     | 1/6     | 1/6     | 1/6     | 1/6     | 1/6     |
| N     | 1/2     | 1/2     | 1/2     | 1/2     | 1/2     | 1/2     | 1/2     | 1/2     | 1/2     | 1/2     | 1/2     | 1/2     | 1/2     |
| N     | 1/6     | 0       | 2/3     | 2/3     | 1/6     | 1/2     | 1/6     | 1/6     | 1/6     | 1/6     | 1/6     | 1/6     | 1/6     |
| N     | 5/6     | 1/2     | 5/6     | 5/6     | 1/2     | 5/6     | 1/2     | 5/6     | 1/2     | 5/6     | 1/2     | 5/6     | 1/2     |

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Table 2: Lattice vectors and fractional coordinates of atoms for the primitive cells used for construction of \{100\}, \{110\}, \{111\}, and \{112\} surfaces of the B3 structure. The N-terminated \{100\} and \{111\} slabs are obtained by exchanging Al and N lattice sites.

|       | \{100\} | \{110\} | \{111\} | \{112\} |
|-------|---------|---------|---------|---------|
| \(\mathbf{a}_1\) | \(1/2\) | \(-1/2\) | \(0\) | \(\sqrt{2}/2\) | \(0\) | \(0\) | \(\sqrt{2}/4\) | \(-\sqrt{6}/4\) | \(0\) | \(\sqrt{3}\) | \(0\) | \(0\) |
| \(\mathbf{a}_2\) | \(1/2\) | \(1/2\) | \(0\) | \(0\) | \(1\) | \(0\) | \(\sqrt{2}/4\) | \(\sqrt{6}/4\) | \(0\) | \(0\) | \(\sqrt{2}/2\) | \(0\) |
| \(\mathbf{a}_3\) | \(0\) | \(0\) | \(1\) | \(0\) | \(0\) | \(\sqrt{2}/2\) | \(0\) | \(0\) | \(\sqrt{3}\) | \(0\) | \(0\) | \(\sqrt{6}/2\) |

Al | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
Al | 1/2 | 1/2 | 1/2 | 1/2 | 1/2 | 1/2 | 1/2 | 1/2 | 1/2 | 1/2 | 1/2 | 1/2 |
Al | 2/3 | 2/3 | 2/3 | 2/3 | 2/3 | 2/3 | 2/3 | 2/3 | 2/3 | 2/3 | 2/3 | 2/3 |
Al | 1/3 | 1/3 | 1/3 | 1/3 | 1/3 | 1/3 | 1/3 | 1/3 | 1/3 | 1/3 | 1/3 | 1/3 |
Al | 0 | 1/2 | 1/2 | 0 | 0 | 3/4 | 0 | 0 | 3/4 | 0 | 0 | 0 |
N | 1/2 | 0 | 3/4 | 0 | 1/4 | 1/2 | 0 | 0 | 0 | 3/4 | 0 | 0 |
N | 0 | 1/2 | 1/4 | 1/2 | 3/4 | 0 | 1/3 | 1/3 | 1/12 | 11/12 | 1/2 | 1/6 |
N | 2/3 | 2/3 | 5/12 | 7/12 | 0 | 1/3 | 0 | 0 | 0 | 0 | 0 | 0 |

Table 3: Lattice vectors and fractional coordinates of atoms for the primitive cells used for construction of \{0001\}, \{1\bar{1}0\}, and \{1\bar{1}2\} surfaces of the B4 structure. The N-terminated \{0001\} slab is obtained by exchanging Al and N lattice sites. \(u\) is the internal parameter describing shift of N atoms above Al sites (\(u_{\text{AIN}} = 0.382\)). \(c\) and \(a\) are the lattice parameters.

|       | \{0001\} | \{1\bar{1}0\} | \{1\bar{1}2\} |
|-------|---------|---------|---------|
| \(\mathbf{a}_1\) | \(1/2\) | \(-\sqrt{3}/2\) | \(0\) | \(1\) | \(0\) | \(0\) | \(3/2\) | \(0\) | \(0\) |
| \(\mathbf{a}_2\) | \(1/2\) | \(\sqrt{3}/2\) | \(0\) | \(0\) | \(c/a\) | \(0\) | \(c/a\) | \(0\) | \(0\) |
| \(\mathbf{a}_3\) | \(0\) | \(0\) | \(c/a\) | \(0\) | \(0\) | \(\sqrt{3}\) | \(0\) | \(0\) | \(\sqrt{3}/2\) |

Al | 1/3 | 2/3 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
Al | 2/3 | 1/3 | 1/2 | 1/2 | 1/2 | 1/2 | 1/2 | 1/2 | 0 | 1/2 | 0 | 1/2 |
Al | 1/2 | 0 | 1/2 | 2/3 | 5/6 | 1/2 | 1/2 | 0 | 0 | 0 | 0 | 0 |
Al | 0 | 1/2 | 2/3 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
N | 1/3 | 2/3 | \(u\) | 0 | \(u\) | 0 | \(u\) | 0 | 0 | 0 | 0 | 0 |
N | 2/3 | 1/3 | 1/2 + \(u\) | 1/2 | 1/2 + \(u\) | 1/2 | 1/2 + \(u\) | 0 | 0 | 0 | 0 | 0 |
N | 1/2 | \(u\) | 1/2 | 1/2 | 1/2 | 1/2 | 1/2 | 0 | 0 | 0 | 0 | 0 |
N | 0 | 1/2 + \(u\) | 2/3 | 5/6 | 1/2 + \(u\) | 1/2 | 1/2 | 0 | 0 | 0 | 0 | 0 |