

Twisted bilayer generator

In order to generate the bilayer we create a supercell for first layer with the cell vectors

$$\begin{aligned}\mathbf{T}_1 &= m\mathbf{a} - n\mathbf{b} \\ \mathbf{T}_2 &= n\mathbf{a} + (m+n)\mathbf{b}\end{aligned}\tag{1}$$

such that $|\mathbf{T}_1| = |\mathbf{T}_2|$. Here m, n are integer numbers, and \mathbf{a}, \mathbf{b} are vectors of the primitive cell.

The total number of the primitive cells in the supercell is

$$N^\theta = m^2 + mn + n^2\tag{2}$$

The cell vectors \mathbf{a}', \mathbf{b}' for the second layer, rotated by angle θ with respect to the first layer:

$$\begin{aligned}\mathbf{a}' &= \mathbf{M}^\theta \mathbf{a} \\ \mathbf{b}' &= \mathbf{M}^\theta \mathbf{b}\end{aligned}\tag{3}$$

where \mathbf{M}^θ is the rotation matrix for angle θ :

$$\mathbf{M}^\theta = \begin{pmatrix} \cos \theta & -\sin \theta \\ \sin \theta & \cos \theta \end{pmatrix}\tag{4}$$

The cell vectors for the supercell for second layer will be

$$\begin{aligned}\mathbf{T}'_1 &= m\mathbf{a}' - n\mathbf{b}' \\ \mathbf{T}'_2 &= n\mathbf{a}' + (m+n)\mathbf{b}'\end{aligned}\tag{5}$$

These vectors should coincide

$$(\mathbf{T}_1, \mathbf{T}_2) = (\mathbf{T}'_1, \mathbf{T}'_2)\tag{6}$$

This condition gives the way to create combined supercell for twisted bilayer.

The relationship between angle θ and m, n is

$$\cos \theta = \frac{m^2 + 4mn + n^2}{2N^\theta}\tag{7}$$

Twisted bilayer for MoS₂

For the primitive cell of MoS₂

$$\begin{aligned}\mathbf{a} &= a(1, 0) \\ \mathbf{b} &= a\left(-\frac{1}{2}, \frac{\sqrt{3}}{2}\right)\end{aligned}\tag{1}$$

here a is the lattice parameter, $a = 3.16 \text{ \AA}$.

The fractional atomic positions in the primitive cell are

$$\text{Mo} = \left(\frac{1}{3}, \frac{2}{3}, 0 \right)$$

$$\text{S} = \left(\frac{2}{3}, \frac{1}{3}, \pm z_0 \right) \quad (2)$$

The distance between the layers $d = 6.15 \text{ \AA}$, whereas the parameter $z_0 = 1.585 \text{ \AA}$.

The possible combinations for m, n for bilayer of MoS₂ generated using Eq. (7) are in the Table

(m, n)	θ (deg)	N (cells/layer)
(2, 1)	21.79	7
(3, 2)	13.17	19
(4, 3)	9.43	37
(5, 3)	9.43	49
(5, 4)	7.34	61
(6, 5)	5.09	91
(7, 6)	3.89	127
(8, 7)	3.14	183
(13, 12)	2.6459	469
(9, 8)	2.60	259
(14, 13)	2.4500	547
(15, 14)	2.2811	631
(16, 15)	2.1339	721
(11, 10)	2.04	331
(17, 16)	2.0046	817
(18, 17)	1.8901	919
(19, 18)	1.7879	1027
(20, 19)	1.6963	1141
(21, 20)	1.6135	1261
(22, 21)	1.5385	1387
(23, 22)	1.4701	1519
(24, 23)	1.4076	1657
(25, 24)	1.3501	1801
(26, 25)	1.2	~2000
(33, 32)	1.0	~3361
(78, 76)	0.8592	17788
(79, 77)	0.8482	18253
(40, 39)	0.8374	4681
(80, 78)	0.8374	18724
(41, 40)	0.8168	4921
(42, 41)	0.7971	5167
(43, 42)	0.7783	5419
(44, 43)	0.7604	5677
(45, 44)	0.7434	5941
(46, 45)	0.7270	6211
(47, 46)	0.7114	6487
(48, 47)	0.6964	6769
(49, 48)	0.6820	7057
(50, 49)	0.6683	7351
(51, 50)	0.6550	7651
(52, 51)	0.6423	7957
(53, 52)	0.6301	8269
(54, 53)	0.6183	8587