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Theory of Wannier orbital

Let us study the theory of most localized Wannier orbital.

Wannier orbitals was introduced many years ago as a method to interpret a band in terms of a bond. Originally this was done by Fourtier transforming the Bloch orbitals with respect to the reciprocal vector. The degree of localization is not sufficient in many cases, requiring thereby stronger localization method. In this context, Prof. Marzari invented an effective procedure.

PDF

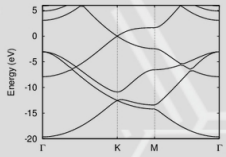

TABLE I. Hopping amplitudes in eV implied by four different **k**-point sampling densities. Intersublattice and intrasublattice amplitudes are grouped separately. The two models on the left, with 5 and 15 parameters, respectively, provide good compromises between accuracy and simplicity.

AB	n	m	N^0	d_n/a	$t_{n,3\times3}$	$t_{n,6\times6}$	$t_{n,12\times12}$	$t_{n,30\times30}$
	1	1	3	$\frac{1}{\sqrt{3}}$	−3.00236	−2.94015	−2.92774	−2.92181
	2	3	3	$\frac{2}{\sqrt{3}}$	−0.22464	−0.26199	−0.27586	−0.27897
	3	4	6	$\sqrt{\frac{7}{3}}$	0.05205	0.03172	0.02807	0.02669
	4	7	6	$\sqrt{\frac{13}{3}}$		−0.00830	−0.00727	−0.00885
	5	8	3	$\frac{4}{\sqrt{3}}$		−0.02463	−0.01812	−0.01772
	6	9	6	$\sqrt{\frac{19}{3}}$		0.00096	0.00463	0.00675
	7	11	3	$\frac{5}{\sqrt{3}}$		0.00467	−0.00227	−0.00262
	8	13	6	$\sqrt{\frac{28}{3}}$		−0.00724	−0.00088	0.00019
	9	14	6	$\sqrt{\frac{31}{3}}$		0.00562	0.00044	−0.00068
	10	16	6	$\sqrt{\frac{37}{3}}$			−0.00230	−0.00237
AA	n	m	N^0	d_n/a	$t'_{n,3\times3}$	$t'_{n,6\times6}$	$t'_{n,12\times12}$	$t'_{n,30\times30}$
	0	0	1	0	0.4770	0.3590	0.3307	0.3208
	1	2	6	1	0.20509	0.21813	0.22377	0.22378
	2	5	6	$\sqrt{3}$	0.06912	0.04357	0.04555	0.04813
	3	6	6	2		−0.02379	−0.02406	−0.02402
	4	10	12	$\sqrt{7}$		0.00538	0.00313	0.00263
	5	12	6	3		0.00783	0.00296	0.00111
	6	15	6	$\frac{6}{\sqrt{3}}$		−0.01429	−0.00110	0.00018
	7	17	12	$\sqrt{\frac{39}{3}}$			−0.00066	−0.00008

For the tight-binding model, please read excellent documents in the web, e.g. the note written by Prof. Fujimori (in Japanese).

次へ

Having learned DFT, let us move to learning program packages. We begin by learning Quantum Espresso

The University of Tokyo

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