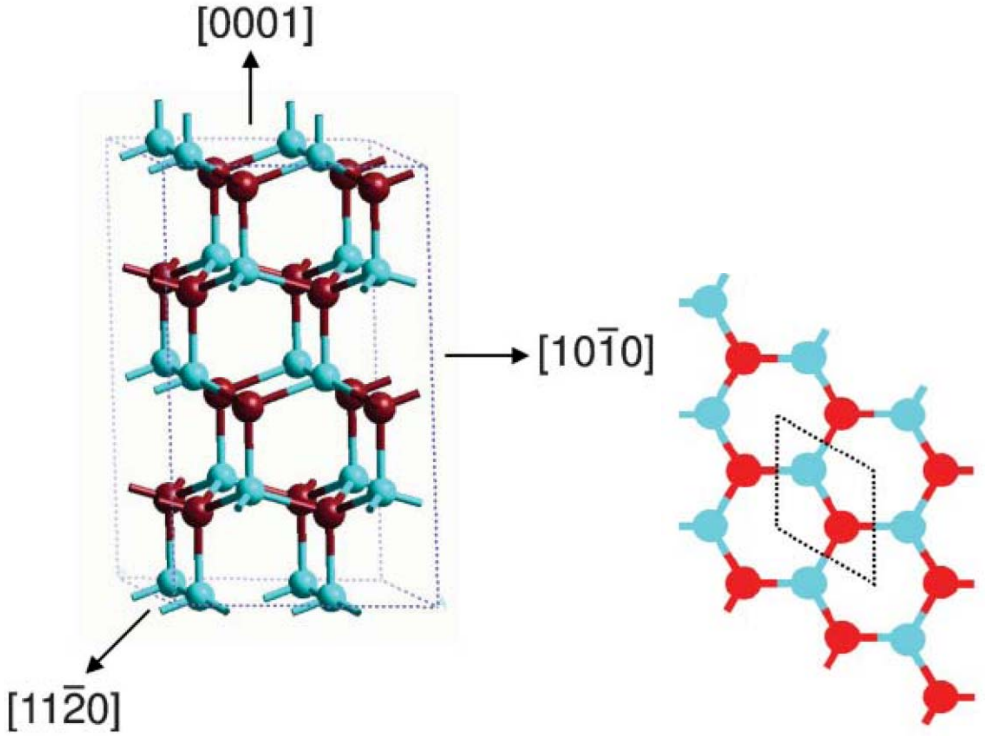
Wurtzite crystal structure. Point group C_{6v}



Character table for point group C_{6v}

C_{6v}	E	$2C_6(z)$	$2C_3(z)$	$C_2(z)$	$3\sigma_v$	$3\sigma_d$	linear functions, rotations	quadratic functions	cubic functions
A_1	+1	+1	+1	+1	+1	+1	z	x^2+y^2, z^2	z^3, $z(x^2+y^2)$
A_2	+1	+1	+1	+1	-1	-1	R_z	-	-
B_1	+1	-1	+1	-1	+1	-1	-	-	$x(x^2-3y^2)$
B_2	+1	-1	+1	-1	-1	+1	-	-	$y(3x^2-y^2)$
E_1	+2	+1	-1	-2	0	0	(x, y) (R_x, R_y)	(xz, yz)	(xz^2, yz^2) [$x(x^2+y^2)$, $y(x^2+y^2)$]
E_2	+2	-1	-1	+2	0	0	-	(x^2-y^2, xy)	[xyz, $z(x^2-y^2)$]

TABLE I. Structure parameters of ZnO crystals.

Authors	Methods	a (Å)	c (Å)	c/a	u
Present	DFT	3.199	5.167	1.615	0.379
Karzel *et al.*[a]	Experiment	3.250	5.204	1.602	0.382
Wu *et al.*[b]	DFT	3.197	5.166	1.616	0.380
Catti *et al.*[c]	Hartree-Fock	3.286	5.241	1.595	0.383

[a]Reference 30.
[b]Reference 35.
[c]Reference 36.

Using the experimental parameters to construct an initial unit cell, we have optimized the structure parameters and summarized them in Table I. Results by other groups are also listed for comparison. It is easy to see that our DFT results are quite close to those of Wu *et al.* and agree well with the experimental results (errors in 2%).

Adopting the optimized structure, we can calculate the elastic constants and piezoelectric coefficients of ZnO crystals. The elastic constants reflect the stress-strain relation of materials. In terms of the symmetry of ZnO crystals (wurtzite structure), this relation can be expressed in the matrix form[37]

$$\begin{bmatrix} \sigma_1 \\ \sigma_2 \\ \sigma_3 \\ \sigma_4 \\ \sigma_5 \\ \sigma_6 \end{bmatrix} = \begin{bmatrix} c_{11} & c_{12} & c_{13} & 0 & 0 & 0 \\ c_{12} & c_{11} & c_{13} & 0 & 0 & 0 \\ c_{13} & c_{13} & c_{33} & 0 & 0 & 0 \\ 0 & 0 & 0 & c_{44} & 0 & 0 \\ 0 & 0 & 0 & 0 & c_{44} & 0 \\ 0 & 0 & 0 & 0 & 0 & \frac{c_{11}-c_{12}}{2} \end{bmatrix} \begin{bmatrix} \epsilon_1 \\ \epsilon_2 \\ \epsilon_3 \\ \epsilon_4 \\ \epsilon_5 \\ \epsilon_6 \end{bmatrix}, \quad (1)$$

where σ_i and ϵ_i $(i=1,\ldots,6)$ represent the stresses and strains, respectively. There are only five independent elastic constants: c_{11}, c_{12}, c_{13}, c_{33}, and c_{44}.

TABLE II. Elastic constants (relaxed ions) of ZnO crystals in units of GPa.

Authors	Methods	c_{11}	c_{12}	c_{13}	c_{33}	c_{44}
Present	DFPT	218	137	121	229	38
Wu *et al.*[a]	DFPT	226	139	123	242	40
Catti *et al.*[b]	Hartree-Fock	246	127	105	246	56
Kobiakov[c]	Experiment	207	118	106	210	45
Azuhata *et al.*[d]	Experiment	190	110	90	196	39

[a]Reference 35.
[b]Reference 36.
[c]Reference 38.
[d]Reference 39.

Similarly, the piezoelectricity can be expressed in the matrix form[37]

$$\begin{bmatrix} P_1 \\ P_2 \\ P_3 - P_3^0 \end{bmatrix} = \begin{bmatrix} 0 & 0 & 0 & 0 & e_{15} & 0 \\ 0 & 0 & 0 & e_{15} & 0 & 0 \\ e_{31} & e_{31} & e_{33} & 0 & 0 & 0 \end{bmatrix} \begin{bmatrix} \epsilon_1 \\ \epsilon_2 \\ \epsilon_3 \\ \epsilon_4 \\ \epsilon_5 \\ \epsilon_6 \end{bmatrix}, \quad (2)$$

where P_1, P_2, and P_3 are three polarization components along the **a** direction, the direction perpendicular to **a** and **c**, and the **c** direction, respectively. P_3^0 is the spontaneous polarization along the **c** direction. There are only three independent piezoelectric coefficients: e_{31}, e_{33}, and e_{15}.

TABLE III. Piezoelectric coefficients (relaxed ions) of ZnO crystals in units of C/m^2.

Authors	Methods	e_{31}	e_{33}	e_{15}
Present	DFPT	−0.65	1.24	−0.54
Wu *et al.*[a]	DFPT	−0.67	1.28	−0.53
Catti *et al.*[b]	Hartree-Fock	−0.55	1.19	−0.46
Kobiakov[c]	Experiment	−0.62	0.96	−0.37

[a]Reference 35.
[b]Reference 36.
[c]Reference 38.

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