The local atomic distribution in tetragonal PZT

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Supplemental Material

TableS1. The lattice parameter a and c, lattice volume, band gap, the softest frequency in gamma point and the zero point energy of supercells.

super cells	a/Å	c/Å	V/Å^3	band gap/eV	softest frequency/cm^{-1}	zero point energy/eV
1	8.9396	8.3886	670.39	2.13216	0.918367	0.120989
2	9.6243	8.7871	813.92	2.18502	-0.642857	0.121929
3	8.3509	7.3330	511.39	2.29956	-0.642857	0.122876
4	8.3510	7.6531	533.72	2.22907	1.43878	0.123854
5	8.2788	7.7128	528.62	2.34361	0.918367	0.121862
6	8.1780	7.1691	479.47	2.31718	-0.642857	0.123801
7	8.9396	8.0038	639.64	2.2467	0.397959	0.122795
8	8.3510	7.5434	526.07	2.39648	0.918367	0.120805
9	9.5922	8.1145	746.62	2.39648	0.918367	0.123715
10	9.5598	8.1685	746.51	2.45815	-1.16327	0.127653
11	8.2788	6.8542	469.78	2.37004	-0.642857	0.127625
12	9.5922	7.6170	700.85	2.48458	-1.16327	0.135501
13	9.5598	7.6512	699.24	2.46696	-2.20408	0.134487
14	9.6243	7.4559	690.61	2.44934	-2.72449	0.136449
15	9.6243	8.4369	781.48	2.36123	-4.28571	0.134434
16	8.2788	7.0264	481.58	2.3348	-3.76531	0.138361
17	8.2788	6.8542	469.78	2.35242	-6.36735	0.14823
18	8.9396	7.8368	626.29	2.21145	-16.2551	0.158082
19	8.3509	7.0875	494.27	2.2467	-14.6939	0.154091
20	9.6243	8.2661	765.66	2.22907	-22.5	0.163951
21	8.3509	6.9471	484.47	1.97357	-18.8571	0.189617
22	8.1780	6.7159	449.16	1.77974	-27.1837	0.266719

The program of crystal generation and statistics:

```
import random
import datetime
#include <iostream>
#include <fstream>
#include <string>
#include <ctime>
#include <vector>
#include <unordered_map>
#include <stdio.h>
#include <stdlib.h>
#include <time.h>

#Defined variable
mx = random.randint(0, 20)
my = random.randint(0, 20)
mz = random.randint(0, 2)

#Generate a crystal structure file
output = "filename
_audit_creation_date                    2024-02-09
_audit_creation_method                  'NJY XATU TRI MCMD'
_symmetry_space_group_name_H-M          'P4mm'
_symmetry_Int_Tables_number             1
_symmetry_cell_setting                  triclinic
loop_
_symmetry_equiv_pos_as_xyz
   x,y,z
_cell_length_a                          80.920
_cell_length_b                          80.920
_cell_length_c                          8.2788
_cell_angle_alpha                       90.0000
_cell_angle_beta                        90.0000
_cell_angle_gamma                       90.0000
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
_atom_site_U_iso_or_equiv
_atom_site_adp_type
_atom_site_occupancy\n"
for mn in range(800):
      atomunit = random.choice(["Zr", "Ti"])
```

```
        output += f"atomunit{mn*5+1}  {atomunit}  {0.5*mx+0.25}  {0.5*my+0.5}  {0.5*mz+0.45170}  uiso  1.00\n"
        output += f"Omn{mn*5+2}  o  {0.5*mx+0.25}  {0.5*my+0.5}  {0.5*mz+0.89730}  uiso  1.00\n"
        output += f"Pbmn{mn*5+3}  o  {0.5*mx}  {0.5*my}  {0.5*mz}  uiso  1.00\n"
        output += f"Omn{mn*5+4}  o  {0.5*mx+0.25}  {0.5*my}  {0.5*mz+0.37850}  uiso  1.00\n"
        output += f"Omn{mn*5+5}  o  {0.5*mx}  {0.5*my+0.5}  {0.5*mz+0.37850}  uiso  1.00\n"

#Output file as*.txt
date_str = datetime.datetime.now().strftime("%Y%m%d")
with open(f"{date_str}_outputcif.txt", "w") as file:
        file.write(output)

#Statistical paragraph information
zrnum = 0
tinum = 0
supercells = []
for mn in range(800):
        if atomunit == "Zr":
                zrnum += 1
        elif atomunit == "Ti":
                tinum += 1

        if mn in [1, 3, 5, 7, 9, 11, 13, 15, 17, 19, 41, 43, 45, 47, 49, 51, 53, 55, 57, 59, 81, 83, 85, 87, 89, 91, 93, 95, 97, 99, 121, 123, 125, 127, 129, 131, 133, 135, 137, 139, 161, 163, 165, 167, 169, 171, 173, 175, 177, 179]:
                supercells.append([output[mn], output[mn+1], output[mn+20], output[mn+21], output[mn+200], output[mn+201], output[mn+220], output[mn+221]])

PZT1 = [Ti.Ti.Ti.Ti.Ti.Ti.Ti.Ti]
PZT2 = [Ti.Ti.Zr.Ti.Ti.Ti.Ti.Ti] or [Zr.Ti.Ti.Ti.Ti.Ti.Ti.Ti]or [Ti.Zr.Ti.Ti.Ti.Ti.Ti.Ti]or [Ti.Ti.Ti.Zr.Ti.Ti.Ti.Ti]or [Ti.Ti.Ti.Ti.Zr.Ti.Ti.Ti]or [Ti.Ti.Ti.Ti.Ti.Zr.Ti.Ti]or [Ti.Ti.Ti.Ti.Ti.Ti.Zr.Ti]or [Ti.Ti.Ti.Ti.Ti.Ti.Ti.Zr]
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PZT4 = [Zr.Ti.Ti.Ti.Ti.Zr.Ti.Ti]or [Ti.Zr.Ti.Ti.Zr.Ti.Ti.Ti]or [Ti.Ti.Zr.Ti.Ti.Ti.Ti.Zr]or [Ti.Ti.Ti.Zr.Ti.Ti.Zr.Ti]or [Zr.Ti.Ti.Zr.Ti.Ti.Ti.Ti]or [Ti.Zr.Zr.Ti.Ti.Ti.Ti.Ti]or [Ti.Ti.Ti.Ti.Zr.Ti.Ti.Zr]or [Ti.Ti.Ti.Ti.Ti.Zr.Zr.Ti]or [Zr.Ti.Ti.Ti.Ti.Ti.Zr.Ti]or [Ti.Ti.Zr.Ti.Zr.Ti.Ti.Ti]or [Ti.Zr.Ti.Ti.Ti.Ti.Ti.Zr]or [Ti.Ti.Ti.Zr.Ti.Zr.Ti.Ti]
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PZT6 = [Zr.Zr.Zr.Ti.Ti.Ti.Ti.Ti]or [Zr.Zr.Ti.Zr.Ti.Ti.Ti.Ti]or [Zr.Ti.Zr.Zr.Ti.Ti.Ti.Ti]or [Ti.Zr.Zr.Zr.Ti.Ti.Ti.Ti]or [Ti.Ti.Ti.Ti.Zr.Zr.Zr.Ti]or [Ti.Ti.Ti.Ti.Zr.Zr.Ti.Zr]or [Ti.Ti.Ti.Ti.Zr.Ti.Zr.Zr]or [Ti.Ti.Zr.Ti.Ti.Zr.Zr.Zr]or [Zr.Zr.Ti.Ti.Zr.Ti.Ti.Ti]or [Zr.Zr.Ti.Ti.Ti.Zr.Ti.Ti]or [Ti.Zr.Ti.Ti.Zr.Zr.Ti.Ti]or [Zr.Ti.Ti.Ti.Zr.Zr.Ti.Ti]or [Ti.Ti.Zr.Zr.Ti.Ti.Zr.Ti]or [Ti.Ti.Zr.Zr.Ti.Ti.Ti.Zr]or [Ti.Ti.Zr.Ti.Ti.Ti.Zr.Zr]or [Ti.Ti.Ti.Zr.Ti.Ti.Zr.Zr]or [Zr.Ti.Zr.Ti.Zr.Ti.Ti.Ti]or [Zr.Ti.Zr.Ti.Ti.Ti.Zr.Ti]or [Ti.Ti.Zr.Ti.Zr.Ti.Zr.Ti]or [Zr.Ti.Ti.Ti.Zr.Ti.Zr.Ti]or [Ti.Zr.Ti.Zr.Ti.Zr.Ti.Ti]or [Ti.Zr.Ti.Zr.Ti.Ti.Ti.Zr]or [Ti.Zr.Ti.Ti.Ti.Zr.Ti.Zr]or [Ti.Ti.Ti.Zr.Ti.Zr.Ti.Zr]

PZT7 = [Ti.Ti.Zr.Zr.Ti.Zr.Ti.Ti]or [Ti.Ti.Zr.Zr.Zr.Ti.Ti.Ti]or [Zr.Zr.Ti.Ti.Ti.Ti.Zr.Ti]or [Zr.Zr.Ti.Ti.Ti.Ti.Ti.Zr]or [Ti.Ti.Zr.Ti.Zr.Zr.Ti.Ti]or [Ti.Ti.Ti.Zr.Zr.Zr.Ti.Ti]or [Zr.Ti.Ti.Ti.Ti.Ti.Zr.Zr]or [Ti.Zr.Ti.Ti.Ti.Ti.Zr.Zr]or [Zr.Ti.Zr.Ti.Ti.Zr.Ti.Ti]or [Zr.Ti.Zr.Ti.Ti.Ti.Ti.Zr]or [Ti.Zr.Ti.Zr.Zr.Ti.Ti.Ti]or [Ti.Zr.Ti.Zr.Ti.Ti.Zr.Ti]or [Ti.Zr.Ti.Ti.Zr.Ti.Zr.Ti]or [Ti.Ti.Ti.Zr.Zr.Ti.Zr.Ti]or [Ti.Ti.Zr.Ti.Ti.Zr.Ti.Zr]or [Zr.Ti.Ti.Ti.Ti.Zr.Ti.Zr]or [Zr.Ti.Ti.Zr.Zr.Ti.Ti.Ti]or [Zr.Ti.Ti.Ti.Zr.Ti.Ti.Zr]or [Ti.Zr.Zr.Ti.Ti.Ti.Zr.Ti]or [Ti.Ti.Zr.Ti.Ti.Zr.Zr.Ti]or [Ti.Zr.Zr.Ti.Ti.Zr.Ti.Ti]or [Ti.Zr.Ti.Ti.Ti.Zr.Zr.Ti]or [Zr.Ti.Ti.Zr.Ti.Ti.Ti.Zr]or [Ti.Ti.Ti.Zr.Zr.Ti.Ti.Zr]

PZT8 = [Ti.Zr.Zr.Ti.Ti.Ti.Ti.Zr]or [Ti.Zr.Zr.Ti.Zr.Ti.Ti.Ti]or [Zr.Ti.Ti.Zr.Ti.Zr.Ti.Ti]or [Zr.Ti.Ti.Zr.Ti.Ti.Zr.Ti]or [Ti.Ti.Zr.Ti.Zr.Ti.Ti.Zr]or [Ti.Zr.Ti.Ti.Zr.Ti.Ti.Zr]or [Zr.Ti.Ti.Ti.Ti.Zr.Zr.Ti]or [Ti.Ti.Ti.Zr.Ti.Zr.Zr.Ti]

PZT9 = [Ti.Zr.Zr.Ti.Zr.Ti.Ti.Zr]or [Zr.Ti.Ti.Zr.Ti.Zr.Zr.Ti]

PZT10 = [Zr.Zr.Ti.Ti.Ti.Ti.Zr.Zr]or [Ti.Ti.Zr.Zr.Ti.Zr.Zr.Ti]or [Zr.Ti.Zr.Ti.Ti.Ti.Zr.Zr]or [Ti.Zr.Ti.Zr.Zr.Ti.Zr.Ti]or [Zr.Ti.Ti.Zr.Zr.Ti.Ti.Zr]or [Ti.Zr.Zr.Ti.Ti.Zr.Zr.Ti]

PZT11 = [Zr.Zr.Zr.Zr.Ti.Ti.Ti.Ti]or [Ti.Ti.Ti.Ti.Zr.Zr.Zr.Zr]or [Zr.Zr.Ti.Ti.Zr.Zr.Ti.Ti]or [Ti.Ti.Zr.Zr.Ti.Ti.Zr.Zr]or [Zr.Ti.Zr.Ti.Zr.Ti.Zr.Ti]or [Ti.Zr.Ti.Zr.Ti.Zr.Ti.Zr]

PZT14 = [Zr.Ti.Zr.Zr.Ti.Ti.Ti.Zr]or [Zr.Ti.Zr.Zr.Zr.Ti.Ti.Ti]or [Ti.Zr.Zr.Zr.Ti.Zr.Ti.Ti]or [Ti.Zr.Zr.Zr.Ti.Ti.Zr.Ti]or [Zr.Zr.Ti.Zr.Zr.Ti.Ti.Ti]or [Zr.Zr.Ti.Zr.Ti.Ti.Ti.Zr]or [Zr.Zr.Zr.Ti.Ti.Ti.Zr.Ti]or [Zr.Zr.Zr.Ti.Ti.Zr.Ti.Ti]or [Ti.Ti.Ti.Zr.Zr.Ti.Zr.Zr]or [Zr.Ti.Ti.Ti.Zr.Ti.Zr.Zr]or [Ti.Zr.Ti.Ti.Ti.Zr.Zr.Zr]or [Ti.Ti.Zr.Ti.Ti.Zr.Zr.Zr]or [Zr.Ti.Ti.Ti.Zr.Zr.Ti.Zr]or [Ti.Ti.Ti.Zr.Zr.Zr.Ti.Zr]or [Ti.Ti.Zr.Ti.Zr.Zr.Zr.Ti]or [Ti.Zr.Ti.Ti.Zr.Zr.Zr.Ti]or [Zr.Zr.Zr.Ti.Ti.Zr.Ti.Ti]or [Zr.Zr.Ti.Ti.Ti.Zr.Ti.Zr]or [Zr.Zr.Ti.Zr.Zr.Ti.Ti.Ti]or [Zr.Zr.Ti.Zr.Ti.Ti.Zr.Ti]or [Zr.Ti.Zr.Ti.Zr.Zr.Ti.Ti]or [Zr.Ti.Ti.Ti.Zr.Zr.Ti.Zr]or [Ti.Zr.Ti.Zr.Zr.Zr.Ti.Ti]or [Ti.Zr.Ti.Ti.Zr.Zr.Zr.Ti]or [Ti.Ti.Zr.Zr.Ti.Zr.Ti.Zr]or [Zr.Ti.Zr.Zr.Ti.Ti.Ti.Zr]or [Ti.Zr.Zr.Zr.Ti.Ti.Zr.Ti]or [Ti.Ti.Zr.Zr.Zr.Ti.Zr.Ti]or [Ti.Ti.Zr.Ti.Ti.Zr.Zr.Zr]or [Zr.Ti.Zr.Ti.Ti.Zr.Zr.Ti]or [Ti.Zr.Ti.Zr.Ti.Zr.Zr.Ti]or [Ti.Ti.Ti.Zr.Zr.Zr.Zr.Ti]or [Zr.Zr.Zr.Ti.Ti.Ti.Zr.Ti]or [Zr.Ti.Zr.Ti.Ti.Ti.Zr.Zr]or [Zr.Zr.Zr.Zr.Ti.Ti.Ti.Ti]or [Zr.Ti.Zr.Ti.Zr.Zr.Ti.Ti]or [Ti.Ti.Zr.Ti.Zr.Zr.Zr.Ti]or [Ti.Ti.Zr.Zr.Zr.Ti.Zr.Ti]or [Zr.Zr.Ti.Ti.Zr.Ti.Zr.Ti]or [Zr.Ti.Ti.Ti.Zr.Ti.Zr.Zr]or [Zr.Zr.Ti.Zr.Ti.Ti.Ti.Zr]or [Ti.Zr.Ti.Zr.Ti.Ti.Zr.Zr]or [Ti.Zr.Zr.Zr.Ti.Zr.Ti.Ti]or [Ti.Zr.Ti.Zr.Zr.Zr.Ti.Ti]or [Ti.Ti.Zr.Zr.Ti.Zr.Ti.Zr]or [Ti.Ti.Ti.Zr.Zr.Zr.Ti.Zr]or [Zr.Zr.Ti.Ti.Ti.Zr.Ti.Zr]or [Ti.Zr.Ti.Ti.Ti.Zr.Zr.Zr]

PZT13 = [Ti.Zr.Zr.Zr.Ti.Ti.Ti.Zr]or [Zr.Zr.Zr.Ti.Zr.Ti.Ti.Ti]or [Zr.Zr.Ti.Zr.Ti.Zr.Ti.Ti]or [Zr.Ti.Zr.Zr.Ti.Ti.Zr.Ti]or [Zr.Ti.Ti.Ti.Zr.Zr.Zr.Ti]or [Ti.Zr.Ti.Ti.Zr.Zr.Ti.Zr]or [Ti.Ti.Zr.Ti.Zr.Ti.Zr.Zr]or [Ti.Ti.Ti.Zr.Ti.Zr.Zr.Zr]

PZT12 = [Ti.Zr.Zr.Zr.Zr.Ti.Ti.Ti]or [Zr.Ti.Zr.Zr.Ti.Zr.Ti.Ti]or [Zr.Zr.Ti.Zr.Ti.Ti.Zr.Ti]or [Zr.Ti.Zr.Zr.Ti.Ti.Ti.Zr]or [Zr.Ti.Ti.Ti.Ti.Zr.Zr.Zr]or [Ti.Zr.Ti.Ti.Zr.Ti.Zr.Zr]or [Ti.Ti.Zr.Ti.Zr.Zr.Ti.Zr]or [Ti.Ti.Ti.Zr.Zr.Ti.Zr.Zr]or [Ti.Zr.Zr.Ti.Zr.Zr.Zr.Ti]or [Zr.Ti.Ti.Zr.Zr.Zr.Ti.Ti]or [Zr.Ti.Ti.Zr.Zr.Ti.Zr.Ti]or [Ti.Zr.Ti.Ti.Zr.Zr.Ti.Zr]or [Zr.Zr.Ti.Ti.Zr.Zr.Ti.Zr]or [Zr.Zr.Ti.Ti.Zr.Ti.Ti.Zr]or [Zr.Ti.Zr.Ti.Zr.Ti.Ti.Zr]or [Ti.Zr.Ti.Zr.Zr.Ti.Ti.Zr]or [Ti.Zr.Zr.Ti.Zr.Ti.Zr.Ti]or [Zr.Ti.Ti.Zr.Zr.Ti.Zr.Ti]or [Zr.Ti.Ti.Zr.Ti.Ti.Zr.Zr]or [Ti.Zr.Ti.Zr.Ti.Ti.Zr.Zr]or [Ti.Ti.Zr.Zr.Ti.Ti.Zr.Zr]or [Zr.Ti.Zr.Ti.Ti.Zr.Zr.Ti]or [Ti.Zr.Ti.Zr.Zr.Ti.Ti.Zr]or [Ti.Ti.Zr.Ti.Zr.Zr.Ti.Zr]or [Zr.Ti.Zr.Zr.Ti.Ti.Zr.Ti]or [Ti.Zr.Ti.Zr.Zr.Ti.Zr.Ti]or [Ti.Ti.Zr.Zr.Ti.Zr.Ti.Zr]

PZT22 = [Zr.Zr.Zr.Zr.Zr.Zr.Zr.Zr]

PZT21 = [Zr.Zr.Ti.Zr.Zr.Zr.Zr.Zr] or [Ti.Zr.Zr.Zr.Zr.Zr.Zr.Zr]or [Zr.Ti.Zr.Zr.Zr.Zr.Zr.Zr]or [Zr.Zr.Zr.Ti.Zr.Zr.Zr.Zr]or [Zr.Zr.Zr.Zr.Ti.Zr.Zr.Zr]or [Zr.Zr.Zr.Zr.Zr.Ti.Zr.Zr]or [Zr.Zr.Zr.Zr.Zr.Zr.Ti.Zr]or [Zr.Zr.Zr.Zr.Zr.Zr.Zr.Ti]

PZT20 = [Zr.Zr.Ti.Ti.Zr.Zr.Zr.Zr]or [Ti.Ti.Zr.Zr.Zr.Zr.Zr.Zr]or [Zr.Zr.Zr.Zr.Ti.Ti.Zr.Zr]or [Zr.Zr.Zr.Zr.Zr.Zr.Ti.Ti]or [Ti.Zr.Ti.Zr.Zr.Zr.Zr.Zr]or [Zr.Ti.Zr.Ti.Zr.Zr.Zr.Zr]or [Zr.Zr.Zr.Zr.Ti.Zr.Ti.Zr]or [Zr.Zr.Zr.Zr.Zr.Ti.Zr.Ti]or [Ti.Zr.Zr.Zr.Ti.Zr.Zr.Zr]or [Zr.Ti.Zr.Zr.Zr.Ti.Zr.Zr]or [Zr.Zr.Ti.Zr.Zr.Zr.Ti.Zr]or [Zr.Zr.Zr.Ti.Zr.Zr.Zr.Ti]

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PZT17 = [Ti.Ti.Ti.Zr.Zr.Zr.Zr.Zr]or [Ti.Ti.Zr.Ti.Zr.Zr.Zr.Zr]or [Ti.Zr.Ti.Ti.Zr.Zr.Zr.Zr]or [Zr.Ti.Ti.Ti.Zr.Zr.Zr.Zr]or [Zr.Zr.Zr.Zr.Ti.Ti.Ti.Zr]or [Zr.Zr.Zr.Zr.Ti.Ti.Zr.Ti]or [Zr.Zr.Zr.Zr.Ti.Zr.Ti.Ti]or [Zr.Zr.Ti.Zr.Zr.Ti.Ti.Ti]or [Ti.Ti.Zr.Zr.Ti.Zr.Zr.Zr]or [Ti.Ti.Zr.Zr.Ti.Ti.Zr.Zr]or [Ti.Zr.Ti.Zr.Zr.Ti.Zr.Zr]or [Zr.Ti.Ti.Zr.Zr.Ti.Zr.Zr]or [Zr.Zr.Ti.Zr.Ti.Zr.Zr.Ti]or [Zr.Zr.Ti.Zr.Zr.Zr.Ti.Ti]or [Zr.Zr.Zr.Ti.Zr.Zr.Ti.Ti]or [Ti.Zr.Ti.Zr.Ti.Zr.Zr.Zr]or [Ti.Zr.Ti.Zr.Zr.Zr.Ti.Zr]or [Zr.Zr.Ti.Zr.Ti.Zr.Ti.Zr]or [Zr.Ti.Zr.Ti.Zr.Zr.Zr.Ti]or [Zr.Ti.Zr.Zr.Zr.Ti.Zr.Ti]or [Zr.Zr.Zr.Ti.Zr.Ti.Zr.Ti]

PZT16 = [Zr.Zr.Ti.Ti.Zr.Ti.Zr.Zr]or [Zr.Zr.Ti.Ti.Ti.Zr.Zr.Zr]or [Ti.Ti.Zr.Zr.Zr.Zr.Ti.Zr]or [Ti.Ti.Zr.Zr.Zr.Zr.Zr.Ti]or [Zr.Zr.Ti.Zr.Ti.Ti.Zr.Zr]or [Zr.Zr.Zr.Ti.Ti.Ti.Zr.Zr]or [Ti.Zr.Zr.Zr.Zr.Zr.Ti.Ti]or [Zr.Ti.Zr.Zr.Zr.Zr.Ti.Ti]or [Ti.Zr.Ti.Zr.Zr.Zr.Zr.Zr]or [Ti.Zr.Ti.Zr.Zr.Zr.Zr.Ti]or [Zr.Ti.Ti.Zr.Ti.Zr.Zr.Zr]or [Zr.Zr.Zr.Ti.Ti.Zr.Ti.Zr]or [Zr.Zr.Zr.Ti.Ti.Zr.Zr.Ti]or [Ti.Zr.Zr.Zr.Zr.Ti.Zr.Ti]or [Ti.Zr.Zr.Ti.Ti.Zr.Zr.Zr]or [Zr.Ti.Ti.Zr.Zr.Zr.Ti.Zr]or [Zr.Zr.Ti.Zr.Zr.Ti.Ti.Zr]or [Zr.Ti.Zr.Zr.Zr.Ti.Ti.Zr]or [Ti.Zr.Zr.Ti.Zr.Zr.Zr.Ti]or [Zr.Zr.Zr.Ti.Ti.Zr.Zr.Ti]

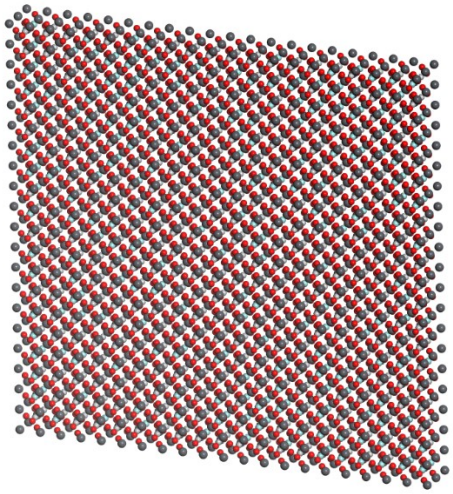
PZT15 = [Zr.Ti.Ti.Zr.Zr.Zr.Zr.Ti]or [Zr.Ti.Ti.Zr.Ti.Zr.Zr.Zr]or [Ti.Zr.Zr.Ti.Zr.Ti.Zr.Zr]or [Ti.Zr.Zr.Ti.Zr.Zr.Ti.Zr]or [Zr.Zr.Ti.Zr.Ti.Zr.Zr.Ti]or [Zr.Ti.Zr.Zr.Ti.Zr.Zr.Ti]or [Ti.Zr.Zr.Zr.Zr.Ti.Ti.Zr]or [Zr.Zr.Zr.Ti.Zr.Ti.Ti.Zr]

```
#Count the number of different supercell arrays
unique_supercells = len(set(map(tuple, supercells)))

#Generate result output
result_output = f"the zr cell's number is{zrnum}      the ti cell's number is{tinum}      the numbe
of different supercell arrays is{unique_supercells}"
with open(f"{date_str}_result_outputrs.txt", "w") as file:
    file.write(result_output)
```

TableS2. The Born effective charge of each central atoms of supercells.

supercell	Zc1	Zc2	Zc3	Zc4	Zc5	Zc6	Zc7	Zc8
1	6.658	6.563	6.736	8.290	8.121	8.486	6.438	6.318
2	9.158	9.147	9.327	10.768	10.547	11.080	8.904	8.692
3	4.554	4.544	4.635	6.210	6.082	6.388	4.488	4.327
4	5.430	5.420	5.528	7.077	6.931	7.281	5.323	5.162
5	5.705	5.694	5.808	7.349	7.198	7.561	5.599	5.410
6	4.563	4.553	4.645	6.215	6.087	6.393	4.496	4.348
7	6.650	6.640	6.771	8.278	8.108	8.517	6.521	6.310
8	4.495	4.485	4.575	6.148	6.022	6.324	4.439	4.272
9	8.483	6.472	6.601	8.112	6.945	8.346	8.328	6.185
10	6.484	6.474	6.602	8.119	7.952	8.354	6.356	6.142
11	3.926	3.915	3.995	5.587	5.472	5.747	3.891	3.726
12	8.104	7.094	7.234	8.934	8.554	8.986	6.636	6.946
13	8.017	7.007	7.164	9.635	8.436	8.914	6.773	7.658
14	7.473	8.915	7.620	9.102	8.482	8.365	6.291	7.131
15	6.763	6.754	6.887	8.397	8.224	8.640	6.627	6.403
16	4.179	4.169	4.253	5.837	5.717	6.004	4.128	3.976
17	4.985	4.976	5.075	6.632	6.495	6.823	4.880	4.770
18	5.690	5.681	5.793	7.333	7.182	7.544	5.602	5.386
19	5.330	5.320	5.426	6.973	6.830	7.174	5.220	5.090
20	7.229	7.220	7.362	8.853	8.671	9.109	7.061	6.873
21	5.503	5.492	5.602	7.150	7.003	7.355	5.351	5.272
22	3.537	3.527	3.599	5.198	5.091	5.346	3.474	3.413



FigS1. The schematic of the computational model of the classical Monte Carlo method.

TableS3. The displacement of each central atoms of supercells.

supercells	Dc1	Dc2	Dc3	Dc4	Dc5	Dc6	Dc7	Dc8
1	0.00509	0.004921	0.4646	0.005023	0.004877	0.5354	0.005264	0.00506
2	0.004752	0.004715	0.5061	0.00496	0.005002	0.5182	0.005149	0.004657
3	0.004665	0.005341	0.5226	0.004776	0.004611	0.468	0.005018	0.004607
4	0.004982	0.004682	0.4842	0.004809	0.005268	0.5097	0.004681	0.005446
5	0.005349	0.005275	0.4784	0.005317	0.004684	0.485	0.004985	0.004641
6	0.004773	0.005427	0.4867	0.005439	0.005011	0.5471	0.005339	0.00511
7	0.004793	0.005039	0.5299	0.004654	0.005176	0.467	0.004912	0.004832
8	0.005229	0.004675	0.5116	0.004601	0.004717	0.5314	0.005077	0.004982
9	0.005112	0.004873	0.4853	0.00541	0.005353	0.4615	0.005235	0.005007
10	0.005071	0.004979	0.5091	0.005023	0.005014	0.4856	0.005444	0.005023
11	0.004976	0.005117	0.4687	0.005022	0.005318	0.471	0.005018	0.005245
12	0.004613	0.004945	0.4679	0.004821	0.005305	0.4913	0.005434	0.005043
13	0.004907	0.004752	0.482	0.004731	0.004809	0.4991	0.004668	0.004985
14	0.0046	0.004671	0.4609	0.005058	0.005197	0.5159	0.005426	0.004699
15	0.005476	0.005432	0.4764	0.005415	0.004776	0.5487	0.004752	0.004635
16	0.005496	0.005086	0.4994	0.005339	0.005273	0.4633	0.00541	0.004619
17	0.005116	0.00477	0.5314	0.005481	0.004855	0.4823	0.004774	0.004925
18	0.00495	0.004821	0.5443	0.004717	0.004924	0.544	0.004689	0.00518
19	0.004713	0.004602	0.5152	0.005149	0.005149	0.486	0.004878	0.005207
20	0.004687	0.00548	0.538	0.005182	0.004863	0.5223	0.005079	0.004983
21	0.005168	0.004832	0.5465	0.005484	0.0049	0.4614	0.00473	0.005113
22	0.00532	0.005185	0.5278	0.004729	0.005418	0.4744	0.004709	0.004715

TableS4. The comparison of Born effective charge in different configurations of supercells.

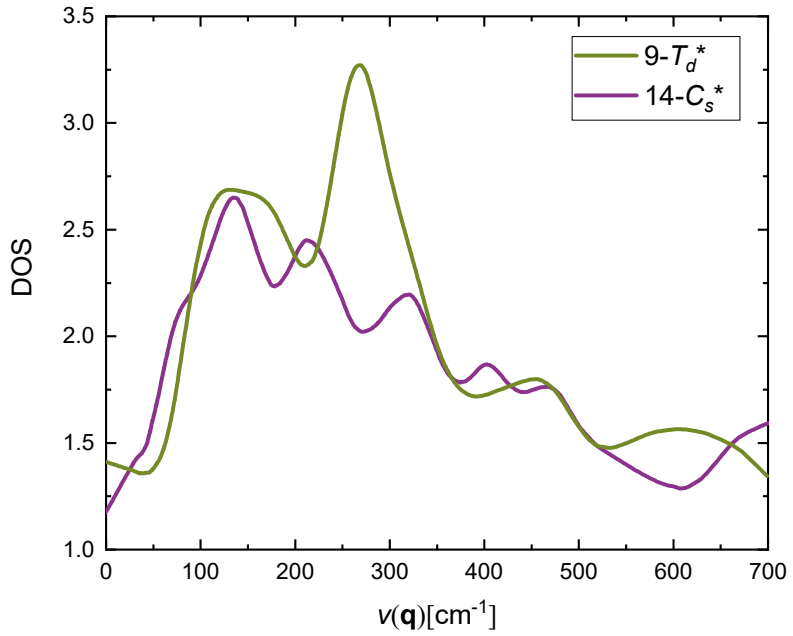
supercells	Zc1	Zc2	Zc3	Zc4	Zc5	Zc6	Zc7	Zc8	softest model frq
3a	4.554	4.544	4.635	6.210	6.082	6.388	4.488	4.327	-0.642857

3b	4.485	4.485	4.533	6.452	6.228	6.279	4.537	4.487	-0.096857128
4a	5.430	5.420	5.528	7.077	6.931	7.281	5.323	5.162	1.43878
4b	5.180	5.545	5.523	6.737	6.848	6.997	5.121	5.100	0.30496388
6a	4.563	4.553	4.645	6.215	6.087	6.393	4.496	4.348	-0.642857
6b	4.454	4.339	4.501	6.345	5.990	6.450	4.325	4.353	-1.29856994
7a	6.650	6.640	6.771	8.278	8.108	8.517	6.521	6.310	0.397959
7b	6.530	6.826	7.096	8.460	7.775	8.338	6.703	6.625	0.243584
10a	6.484	6.474	6.602	8.119	7.952	8.354	6.356	6.142	-2.20408
10b	6.497	6.163	6.404	8.282	7.976	8.696	6.051	6.142	-1.9085552
11a	3.926	3.915	3.995	5.587	5.472	5.747	3.891	3.726	-2.72449
11b	4.118	3.802	3.891	5.593	5.450	5.615	4.019	3.838	-1.82529613
12a	7.104	7.094	7.234	8.734	8.554	8.986	6.936	6.746	-1.16327
12b	7.069	7.016	7.155	9.066	8.922	9.229	6.631	6.456	-2.11906574
14a	7.482	7.473	7.620	9.102	8.915	9.365	7.291	7.131	-1.16327
14b	7.714	7.622	7.734	9.238	8.745	8.991	7.532	7.209	-1.11092285
16a	4.179	4.169	4.253	5.837	5.717	6.004	4.128	3.976	-3.76531
16b	4.263	4.202	4.219	5.714	5.757	5.848	4.252	4.131	-2.94981019
17a	4.985	4.976	5.075	6.632	6.495	6.823	4.880	4.770	-6.36735
17b	5.055	5.115	5.242	6.320	6.599	6.980	4.846	4.546	-2.1635948
19a	5.330	5.320	5.426	6.973	6.830	7.174	5.220	5.090	-14.6939
19b	5.229	5.570	5.513	7.224	6.857	7.439	5.283	5.156	-21.253083
20a	7.229	7.220	7.362	8.853	8.671	9.109	7.061	6.873	-22.5
20b	7.583	7.583	7.384	9.048	8.740	8.790	6.708	7.154	-18.1075

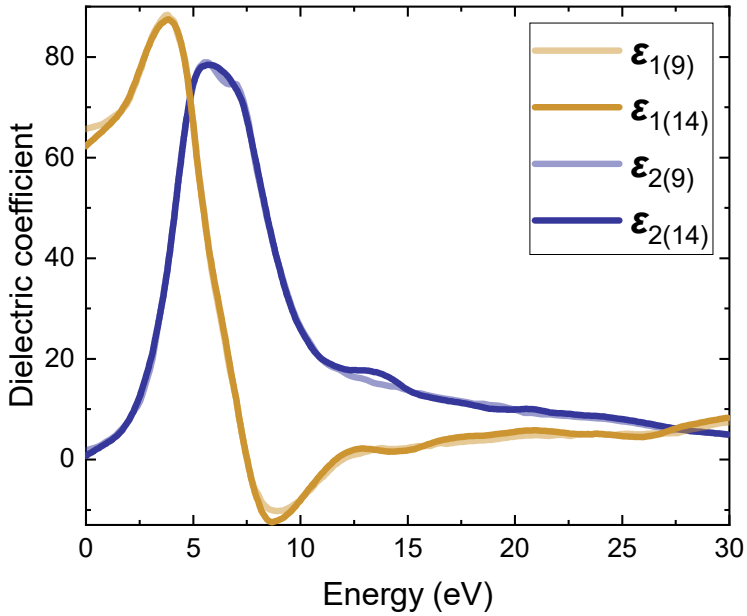
TableS5. The Born effective charge and softest frequency of Rhombohedral supercells.

supercells	Zc1	Zc2	Zc3	Zc4	Zc5	Zc6	Zc7	Zc8	softest model frq
1	7.358	7.358	7.358	7.358	7.358	7.358	7.358	7.358	1.74955648
2	8.112	7.579	7.991	8.112	7.634	7.921	8.112	7.889	1.50640266
3a	8.296	8.296	7.883	7.883	8.259	8.259	8.296	8.271	0.331190774
3b	8.365	8.365	7.946	7.946	8.327	8.327	8.365	8.340	0.32539646
4a	7.604	7.932	7.397	7.412	7.856	7.604	7.412	7.624	-0.738642693
4b	7.662	7.995	7.452	7.467	7.917	7.662	7.467	7.682	-1.466085462
5	7.760	7.760	7.425	7.760	7.760	7.425	7.760	7.648	-1.533611099
6a	8.203	7.534	7.875	8.753	7.221	8.401	8.753	8.125	0.405520221
6b	8.270	7.591	7.937	8.830	7.273	8.472	8.830	8.191	0.307159424
7a	7.467	8.682	7.415	7.576	8.445	8.434	7.820	8.233	0.272326912
7b	7.523	8.757	7.470	7.633	8.516	8.505	7.881	8.301	-2.67134496
8	8.045	8.405	8.405	7.864	7.333	7.381	8.405	7.706	-2.061239616
9	7.732	7.939	7.939	7.732	7.939	7.732	7.732	7.801	-3.52276557
10a	8.215	8.215	8.627	8.627	8.627	8.627	8.215	8.490	-2.79532674
10b	8.283	8.283	8.701	8.701	8.701	8.701	8.283	8.562	-2.191113975
11a	8.584	8.584	8.584	8.584	7.953	7.953	7.953	7.953	-2.361933192
11b	8.658	8.658	8.658	8.658	8.017	8.017	8.017	8.017	-1.37149533

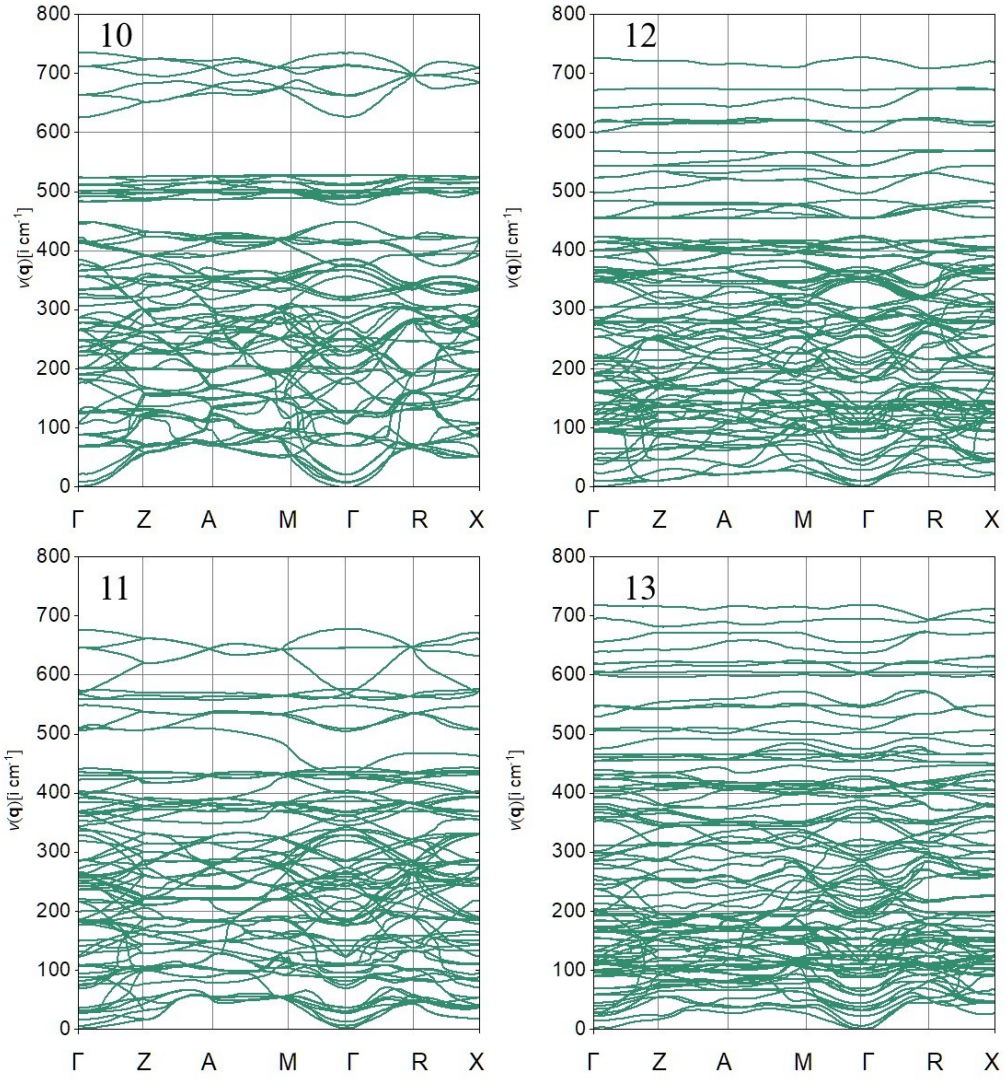
12a	8.507	8.460	8.976	8.807	8.939	9.190	8.814	8.981	-1.4308221
12b	8.580	8.532	9.056	8.884	9.019	9.275	8.892	9.062	-2.280114736
13	8.804	9.217	9.384	9.213	8.381	9.262	9.569	9.070	-4.16066755
14a	9.450	8.855	9.154	8.381	9.282	8.684	9.335	9.100	-1.42151594
14b	9.540	8.933	9.237	8.451	9.368	8.760	9.422	9.183	-1.227569749
15	8.827	8.397	8.397	8.940	8.397	7.882	8.974	8.418	-3.584019381
16a	8.556	8.374	7.875	8.628	8.327	8.714	8.604	8.548	-4.60497413
16b	8.629	8.444	7.937	8.703	8.396	8.790	8.679	8.621	-6.56473785
17a	8.498	8.524	8.738	8.638	8.774	9.042	8.638	8.818	-3.772807233
17b	8.570	8.597	8.814	8.712	8.851	9.124	8.712	8.896	-6.45012555
18	7.955	7.955	8.503	7.955	7.955	8.503	7.955	8.137	-2.54655108
19a	8.766	8.150	8.826	8.829	8.041	8.766	8.829	8.545	-2.399426633
19b	8.843	8.216	8.904	8.907	8.106	8.843	8.907	8.618	-18.4849262
20a	8.670	8.670	7.718	7.718	8.564	8.564	8.670	8.599	-15.1787987
20b	8.746	8.746	7.777	7.777	8.637	8.637	8.746	8.673	-23.93097146
21	8.555	8.944	9.073	8.555	8.503	8.141	8.555	8.400	-28.7775
22	7.634	7.634	7.634	7.634	7.634	7.634	7.634	7.634	-17.4358515



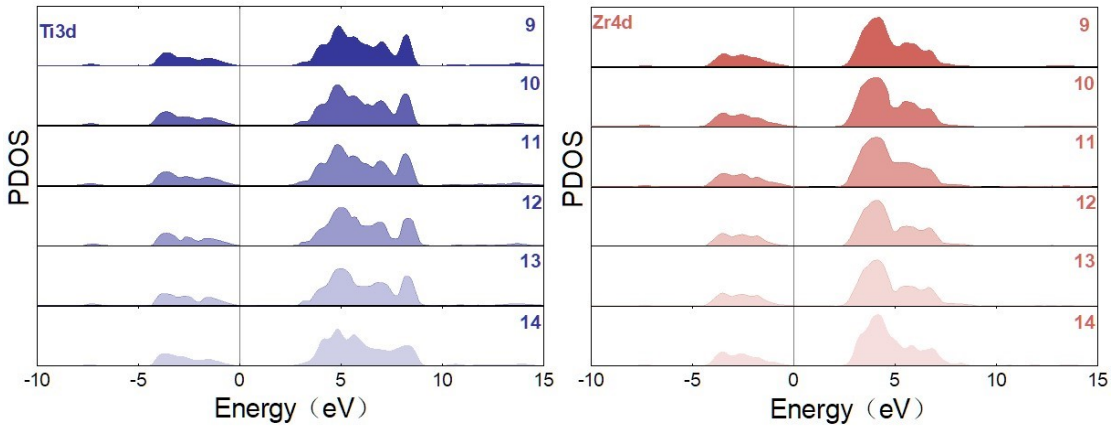
FigS2. Density of phonon states of the supercell 14 and 9.



FigS3. Real (ε_1) and imaginary (ε_2) components of the complex dielectric function of the supercell 14 and 9.



FigS4. Phonon scattering spectra of the supercells near MPB. (layered-types: 10, 11; these mixed-types: 12, 13)



FigS5. The Compare of density of states of layered-types and mixed-types.