

## Evaluate the piezoelectric properties of $\text{Li}_{1-x}\text{Na}_x\text{NbO}_3$ by first-principles calculation

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### Introduction

In recent years, our laboratory has reported the piezoelectric  $\text{LiNbO}_3$  provides a multi-piezo material that combines mechanoluminescence (ML) properties and piezoelectric properties by doping  $\text{Pr}^{3+}$  [1]. The piezoelectricity properties of  $\text{LiNbO}_3$ :  $\text{Pr}^{3+}$  changing with the addition of Na has been reported and it also shows a strong relationship between ML intensity and piezoelectricity [2]. To study the relationship between its piezoelectricity and ML, the evaluation of its piezoelectricity is essential. However, without the addition of  $\text{Pr}^{3+}$ , the piezoelectricity-related data of  $\text{Li}_{1-x}\text{Na}_x\text{NbO}_3$  are still insufficient. In this study the first-principles calculation was used to investigate the piezoelectricity of  $\text{Li}_{1-x}\text{Na}_x\text{NbO}_3$ .

### Calculation Method

The Vienna Ab Initio Simulation Package (VASP) was used to calculate the changes of physical properties with the amount of sodium increase. The supercell of  $\text{Li}_{1-x}\text{Na}_x\text{NbO}_3$  was made by special quasirandom structure method. Density Functional Perturbation Theory method and Frozen Phonon method was used to calculate the piezoelectric stress constant ( $e_{33}$ ) and elastic constant ( $C_{33}$ ). The piezoelectric constant ( $d_{33}$ ) was calculated by using  $e_{33}$  and  $C_{33}$ .

### Results And Discussion

Figures 1 and 2 show the calculated results of the elastic constant  $C_{33}$  and the piezoelectric stress constant  $e_{33}$  with respect to the amount of Na added in  $\text{Li}_{1-x}\text{Na}_x\text{NbO}_3$ . As the addition of Na increases,  $e_{33}$  increases first and then decreases and reaching the maximum when  $\text{Na}=0.9$ ,  $C_{33}$  decreases gradually. By compared the calculated value and experiment value of  $e_{33}$  and  $C_{33}$  at  $\text{LiNbO}_3$ , it is confirmed that the calculated results have high reliability. Calculated  $d_{33}$  value, it increases first and then decreases with Na increase, and the trend is consistent with the experiment.

### References

[1] D. Tu, etc. Adv Mater, 29.22 (2017). [2] H. Hara, etc. Soc. J., 128,518-522 (2020).

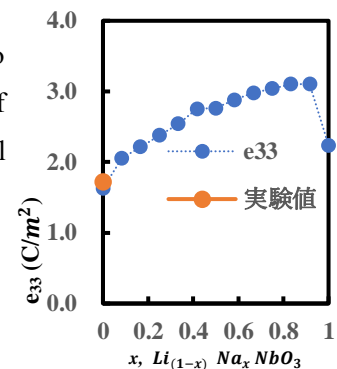


Figure.1 Calculated piezoelectric constant.

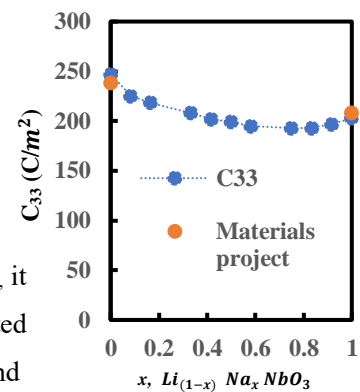


Figure.1 Calculated elastic constant.