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Electronic and optical properties of co-doped BaTi O_3 with fluorine and nitrogen: A first-principles study. JAWAD ALSAEI[1], Universit of Bahrain, PUAL TANGNEY, ARASH MOSTOFI, Imperial College London — Ferroelectric oxides such as BaTi O_3 (BTO) are very good candidates for tunable dielectric devices. Tailoring the electronic and optical properties of these materials is usually achieved through means of strain engineering and compositional variations. In this work, we use first-principles calculations to study the effect of the co-substitution of F and N in BTO on its electronic and optical properties. Our simulations suggest that the optical properties are very sensitive to the atomic configuration of the dopant atoms. Our simulations show that the most energetically favorable configuration is that in which the F and N atoms form linear parallel chains of F-Ti-N motif that tend to cluster with each other. This configuration induces a large birefringence that can be further enhanced by means of biaxial strain. Our results shed more light on this particular type of anionic doping that has been rarely studied in the literature [**?**].

References

[1] Kumar, N., Pan, J., Aysha, N., Waghmare, U. V., Sundaresan, A., and Rao, C. (2013) Journal of Physics: Condensed Matter 25(34), 345901.

[1]This work has been done while J. Alsaei was at Imperial College London.

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