Research Statement

Perovskites are a family of crystal structures which are at the forefront of scientific interest due to the wide variety of properties, and thus applications, that they have been observed to exhibit. In particular, sodium niobate-based perovskites show promising electronic properties such as antiferroelectricity and piezoelectricity, leading to many applications from optical storage to sensors and actuators. Perovskites' properties are highly variable depending on the exact molecular makeup of the crystal, and so a thorough understanding of possible structures of both end member perovskites (e.g. $NaNbO_3$ or $KNbO_3$) and partially substituted perovskites (e.g. $Na_xK_{1-x}NbO_3$) is key to the industrial development of technologies in this area.

Due to the high oxygen content and the short-range order of these mixed metal niobate-based perovskites, these would ideally be investigated using ^{17}O NMR. NMR analysis is used to find each type of environment a type of atom is exposed to – i.e. ^{17}O atoms. The ^{17}O isotope is, however, of very low natural abundance of 0.037% and the isotopic enrichment necessary is very costly. Thus, current research has been investigating the use of computational calculations in order to simulate ^{17}O NMR in order to make this research much more sustainable.

This research project bases itself off these considerations. Firstly, density functional theory calculations will be applied to the end member perovskites $NaNbO_3$, $KNbO_3$ and $LiNbO_3$ using two different methods called functionals (PBE and PBEsol) and the results compared to literature values in order to evaluate the accuracy of the calculations. Then, low level substitution of potassium and lithium into $NaNbO_3$ will be investigated to yield parameters needed for NMR as well as mixing energies. The system is then modelled to look at the possible configurations of the system, while streamlining equivalent configurations, in order to improve the output of the NMR simulation. The NMR simulations will be carried out for ^{23}Na, ^{39}K and ^{17}O and compared with literature.