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Substitution site for Zn in $LiNbO_3$ from detailed EXAFS analysis[1]
FRANK BRIDGES, BRAD CAR, UCSC, JAIME CASTILLO, Universidad Tecnologica d la Mixteca, MICHAEL KOZINA, SCOTT MEDLING, UCSC — We report detailed EXAFS studies of Zn doped $LiNbO_3$, at the Zn and Nb K-edges, as a function of dopant and as a function of temperature. For this material there exist several models concerning the substition site(s) for Zn. Our data are only consistent with Zn substitution on the Li site. Any substitution on the Nb site is very small. Further as the Zn concentration changes from 5-9% the EXAFS r-space function for the Zn K-edge changes very little, a slight amplitude reduction consistent with increased local disorder for increasing Zn concentration. Our detailed analysis shows that the nearest O neighbors to Zn are slightly pulled inward while the nearst metal atoms - Nb - are pushed away. We cannot tell if there are vacancies on the Li sites because Li is a very weak backscatterer, and the amplitude of the rather long Zn-Li peak is very low. We discuss and compare our results with previous proposed models and with recent calculations for other defects that suggest that many +2 dopants substitute at the Li site.

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