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Argon removal from liquid nitrogen using zeolites

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Liquid nitrogen produced underground is contaminated with other elements, most prominently 3.6% argon. Argon is slightly radioactive, which increases the background for the SNO+ experiment, and has a higher freezing point (84 K) than nitrogen, which creates problems as DEAP and nEXO plan to use liquid nitrogen for cooling. Zeolites are a low-cost solution to filter out argon from liquid nitrogen. Zeolites are aluminosilicates with different framework types and are used as molecular sieves to filter out specific molecules. For this project we use the Linde Type A (LTA) framework with silver in the center of the LTA cages since it is beneficial to use cations with large, polarizable electron clouds. Simulation work was done using CP2K, a molecular dynamics software based on Fortran. Exploratory simulations involving geometry optimization of the LTA zeolite unit cells with different cations in the center were conducted. Various molecular dynamics simulations of LTA zeolites with dimensions of 3x3x3 and 4x4x10 angstroms were also done to investigate the slowing capacity of the zeolites. In this talk, I will be presenting the results of these simulations.

What area of study best describes your talk?

Physics

If you answered 'Other', please provide the study area.

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