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Ba^{2+}-Xe_n Clustering and Subsequent Mobility in ^{136}Xe Gas EDAN BAINGLASS, BENJAMIN JONES, DAVID NYGREN, MUHAMMAD HUDA[1], University of Texas Arlington — The possibility of clustering between Ba^{2+} and ^{136}Xe gas has been investigated as part of a neutrinoless double beta decay ($0\nu\beta\beta$) detection experiment. The success of the experiment depends in part on the ability of Ba^{2+} to drift along an imposed electric field towards a detector. The question of clustering was raised due to the highly ionized Ba^{2+} daughter isotope and its potential of inducing dipoles in the surrounding ^{136}Xe gas. Such clustering would alter the mass and effective charge of the particle, thus changing the dynamics of the experiment. Density Functional Theory was employed in producing the potential energy surface for Ba^{2+}-Xe dimer. The Ba^{2+} ion was modeled by a modified Gaussian basis set to account for the high ionization. Utilizing the modified basis set, clustering for $BaXe_n$ (n=2-10) was investigated at 300K and was found to have the highest stability at $BaXe_3$. A Monte Carlo simulation was developed to obtain the drift velocity and derive the mobility coefficient K_0 as a function of operating perimeters. Results and algorithms will be presented.

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