

The thermophysical properties of nuclear fuels being developed in generation IV nuclear reactors are still being widely examined since the reactor's operating performance is strongly correlated to the thermal transport properties of the fuel source. In this research, phonon density of states (DOS) are estimated for uranium dioxide ( $\text{UO}_2$ ), thorium dioxide ( $\text{ThO}_2$ ), and plutonium dioxide ( $\text{PuO}_2$ ) as these are all significant representations of the actinide oxide family. The crystalline structures of these fuels are altered to contain point defects in the form of primary atom vacancies, oxygen vacancies, and uranium substitution. Primary atom and oxygen vacancies involve a set percentage (0.1%, 0.5%, 1%, 2%, and 5%) of atoms being removed from the lattice structure of each fuel, while the uranium substitution in  $\text{ThO}_2$  and  $\text{PuO}_2$  replaces a set percentage of primary atoms with uranium-238 atoms. Phonon DOS are plotted using molecular dynamics simulations and the Fourier transform of the velocity autocorrelation function of atoms. The results show that phonon DOS is altered greatly by the presence of any form of vacancy defects; a significant change in DOS is observed in low frequency regime ( $\sim 20$  meV) where most of important energy carriers (phonons) are activated, and this explains the significant reduction in thermal conductivity in nuclear fuels by vacancy defects. Also, it is found that the change in phonon DOS by oxygen vacancies is smaller than that by primary atom vacancies, supporting our previous results that showed that the thermal conductivity is reduced by primary atom vacancies more than by oxygen vacancies. The most interesting observation is made on nuclear fuels with uranium substitution that shows very little variance in phonon DOS; the very small decrease in the thermal conductivities of  $\text{PuO}_2$  and  $\text{ThO}_2$  by uranium substitution results from their minimal alteration to lattice vibration.