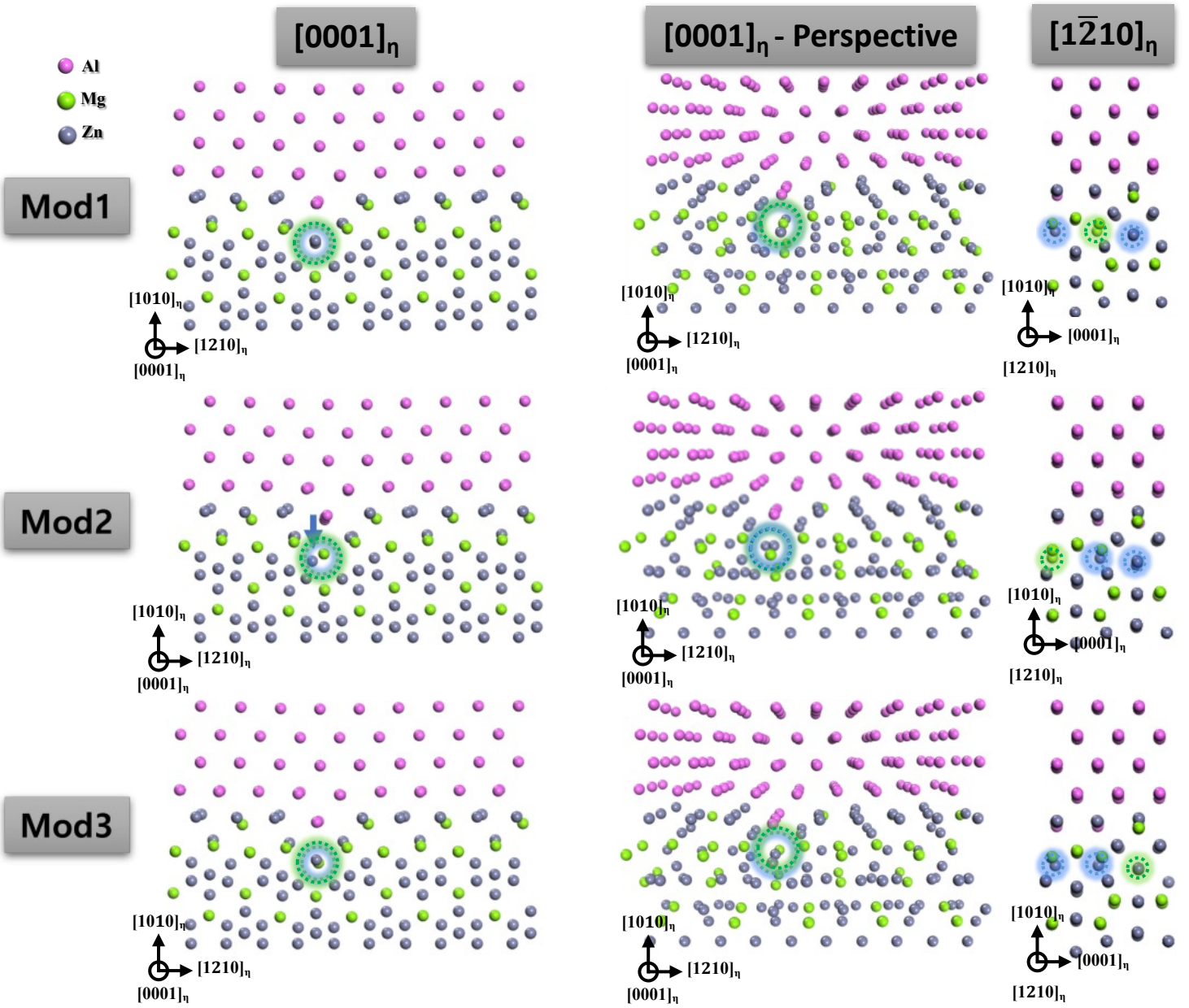
Supplementary figure 1. Three different candidate atomic models with different Mg position along $[0001]_\eta$ direction after atomic structure relaxation. Pink atom indicates Al, green atom indicates Mg and grey atom indicates Zn. Blue dotted circle shows Zn atom site and green dotted circle shows Mg atom site. Among these three models, Mod3 is in a good agreement with experimental result.



Supplementary figure 2. Total energy calculation result of three different candidate atomic models shown in supplementary figure 1. Among these three models, Mod3 was energetically favored.