A DFT STUDY OF THE STRUCTURE AND PROPERTIES OF NITROGEN DOPING SPINEL
MgAl\textsubscript{2}O\textsubscript{3.5}N\textsubscript{0.5}

P. K. Leong\textsuperscript{1}, C. P. Tang\textsuperscript{1}, S. I. Tam\textsuperscript{1} and T. Sekine\textsuperscript{2}, \textsuperscript{1}State Key Laboratory of Lunar and Planetary Sciences, Macau University of Science and Technology, Macau. E-mail: cptang@must.edu.mo, \textsuperscript{2}Center for High Pressure Science and Technology Advanced Research (HPSTAR) Shanghai Laboratory of HPSTAR, Shanghai, P.R. China. E-mail: toshimori.sekine@hpstar.ac.cn

**Introduction:** Since spinel has an important role of planetary composition, doped spinels are also studied for their properties\cite{1-3} (electronic, optical, magnetic, etc.) in astronomical implications.\cite{4} In this work, we report a possible nitrogen-doped oxygen structure of spinel with density functional theory (DFT). The studies of the structural and electronic properties (band structure, density of states and phonon) of the spinel (MgAl\textsubscript{2}O\textsubscript{4}) and the N doping spinel (MgAl\textsubscript{2}O\textsubscript{3.5}N\textsubscript{0.5}) compounds are performed using the generalized gradient approximation and the Perdew-Burke-Ernzerh of (GGA/PBE) functional. The density and space group (in brackets) of the two crystal cells are 3.47 g/cm\textsuperscript{3} (Fd\textsubscript{3}m) for MgAl\textsubscript{2}O\textsubscript{4} and 3.38 g/cm\textsuperscript{3} (R\textsubscript{3}m) for MgAl\textsubscript{2}O\textsubscript{3.5}N\textsubscript{0.5}, respectively. The calculated direct band gaps at the \textit{\Gamma}-point are approximately 5.13 eV for MgAl\textsubscript{2}O\textsubscript{4} and 4.24 eV for MgAl\textsubscript{2}O\textsubscript{3.5}N\textsubscript{0.5}. The density of states analysis shows that the tops of the valence bands are constituted \textasciitilde93\% of the p(O) states and \textasciitilde60\% of p(N) + \textasciitilde32\% of p(O) states (for MgAl\textsubscript{2}O\textsubscript{4} and MgAl\textsubscript{2}O\textsubscript{3.5}N\textsubscript{0.5}, respectively). In the phonon analysis, the lowest frequency of MgAl\textsubscript{2}O\textsubscript{3.5}N\textsubscript{0.5} is redshifted to 36.6 cm\textsuperscript{-1} (MgAl2O4 is 39.8 cm\textsuperscript{-1}) caused by the N-doped. Finally, we calculated the cohesive energy dependence for the pressure of the two spinels. We found that the cohesive energy of MgAl\textsubscript{2}O\textsubscript{3.5}N\textsubscript{0.5} is lower than MgAl\textsubscript{2}O\textsubscript{4} when the pressure is higher than \textasciitilde115 GPa. It implies that MgAl\textsubscript{2}O\textsubscript{3.5}N\textsubscript{0.5} is more stability than MgAl\textsubscript{2}O\textsubscript{4} at high pressure. Base on these results, we suggest that nitrogen atom would replace the oxygen of spinel in the depths of the earth or other planets.