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Phonon frequencies, Born effective charges and LO-TO splitting of *Mg*-IV-N_2 semiconductors

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Mg-IV-N_2 semiconductors, with the group-IV (Si, Ge, and Sn), are alternative materials beside a series of III-N, e.g. AlN, GaN and InN, which is used widely for optoelectronic devices. This work presents phonon frequencies, Born effective charges and longitudinal optical - transverse optical (LO-TO) splitting of these compounds at gamma point by using the density-functional perturbation theory. We employ the norm-conserving pseudopotential within the generalized gradient and the local-density approximation as implemented in ABINIT package. The results are compared with Cd-IV- N_2 and Zn-IV- N_2 semiconductors to predict the phonon property trend of II-IV- N_2 series.

Authors: Mr KAEWMEECHAI, Chaiyawat; Dr PUNYA JAROENJITTICHAI, Atchara

Presenter: Mr KAEWMEECHAI, Chaiyawat

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