Electronic properties of MA_2Z_4 family of layered 2D materials

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Layered MA_2Z_4 family of materials has recently drawn a great interest as a promising class of 2D semiconductors, due to their exceptional electronic and mechanical properties [1]. For instance, $MoSi_2N_4$ and WSi_2N_4 monolayers have been successfully synthesized using chemical vapor deposition, however, many more members of this material's family were predicted theoretically [2]. Motivated by this research, we have explored the electronic properties of this new family of layered 2D materials. In this work, we systematically investigated the MA_2Z_4 (M = Mo, W; A = Si; Z = N, P, As, Sb) monolayers in pure form as well as mixed forms, with two different Z elements in the same layer, using density functional theory (DFT) calculations. Phonon dispersion relation showed that most of the models are stable. The band decomposed charge densities were plotted for these monolayers, showing localization of electron and hole states (see Figure 1) The exciton g-factors from first principles, which can be measure experimentally, were also calculated for all possible spin-valley configurations of excitons in a monolayer. The theoretical aspect of our work provides insights into the future nano(opto)electronic applications of MA_2Z_4 monolayers.

References

[1] Hong, Yi-Lun, et al., Science, 369.6504 (2020): 670-674.
[2] Wu, Qingyun, et al., *Applied Physics Letters*, 118.11 (2021): 113102.

Figures

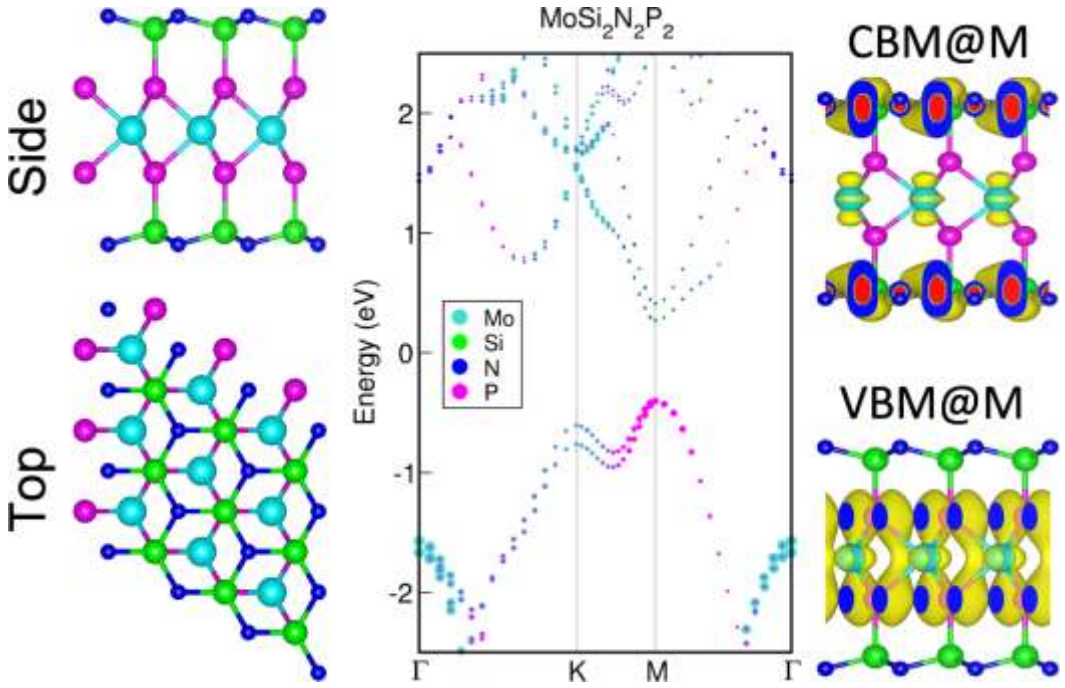

Figure 1: Structure, electronics and band decomposed charge densities of $MoSi_2N_2P_2$ monolayer.