chem2Dmat
AUGUST 31 - SEPTEMBER 03, 2021 • ONLINE

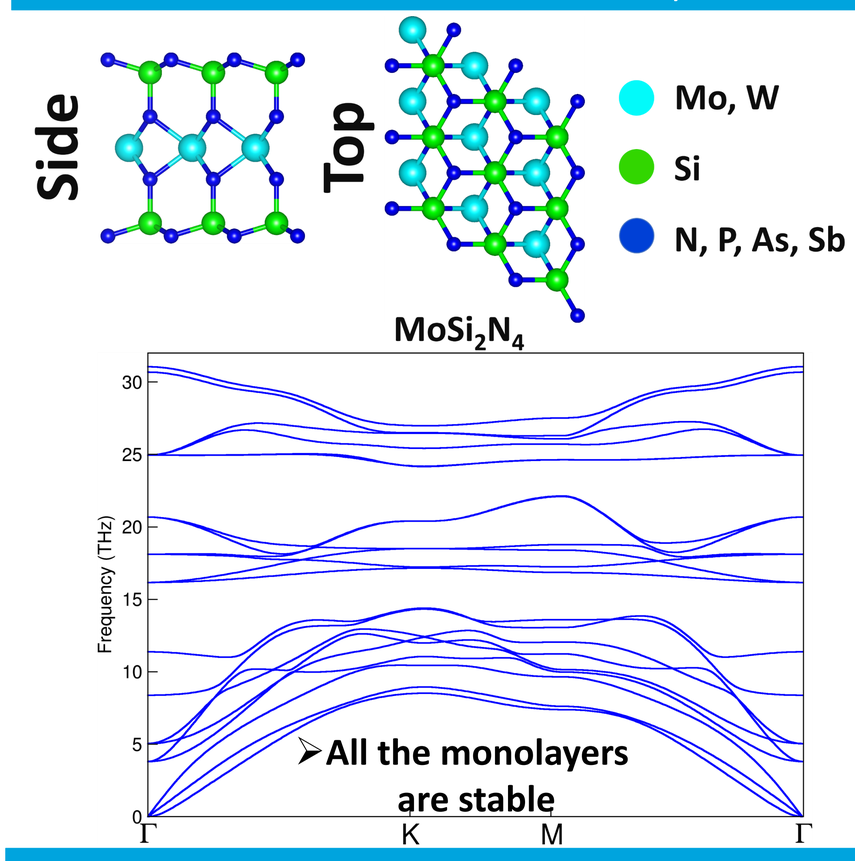
Electronic properties of MA_2Z_4 family of layered 2D materials

Umm-e-Hani,[1] Muhammad Sufyan Ramzan,[1,2] Tomasz Woźniak,[3] Agnieszka Kuc[1,2]
[1] Jacobs University Bremen gGmbH, Campus Ring 1, 28759 Bremen, Germany
[2]Helmholtz-Zentrum Dresden-Rossendorf, Institute of Resource Ecology, Permoserstrasse 15, 04103 Leipzig, Germany
[3]Department of Semiconductor Materials Engineering, wyb. Wyspiańskiego 27, 50-370 Wrocław, Poland
u.asghar@jacobs-university.de

Abstract

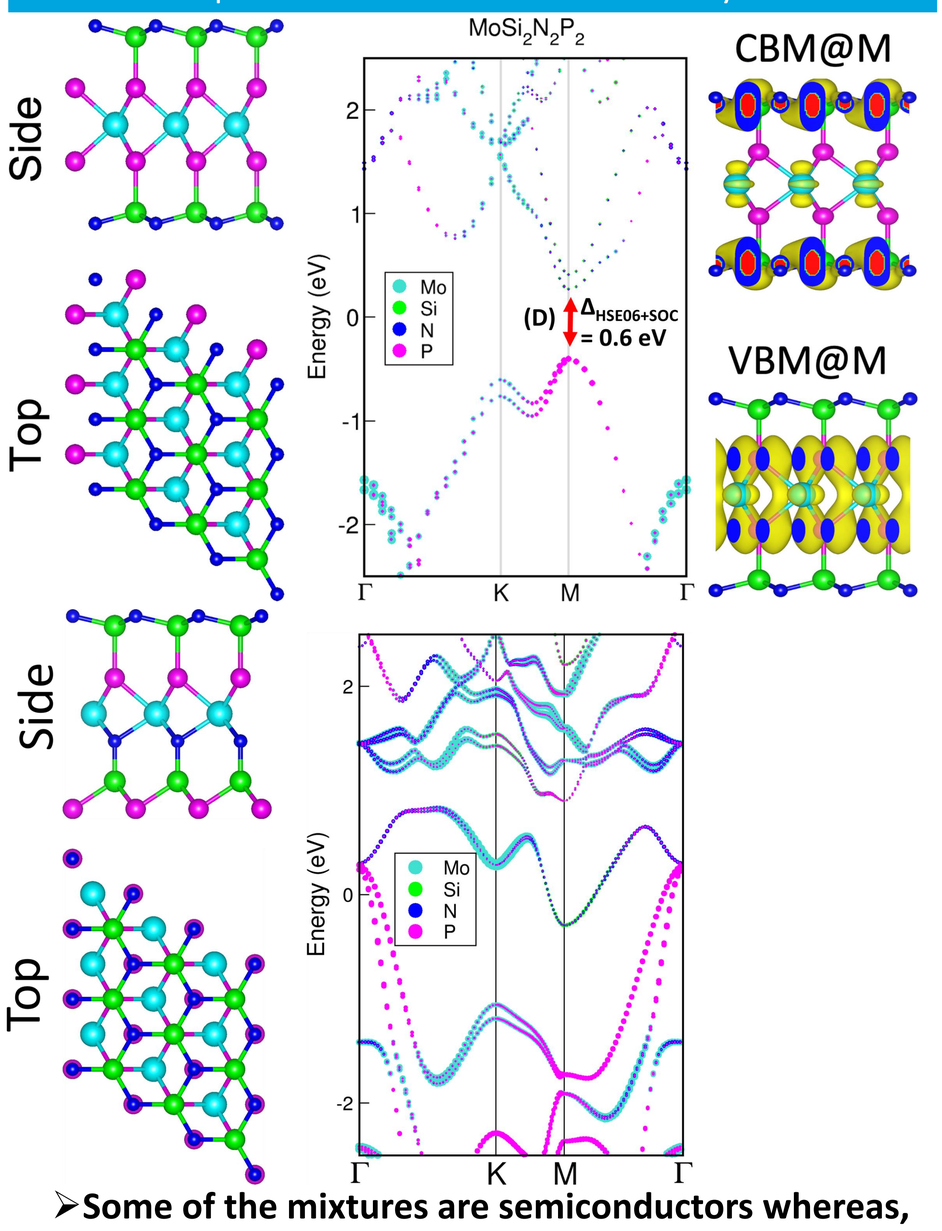
Layered MA_2Z_4 family of materials has recently drawn a great interest as a promising class of 2D semiconductors, due to their exceptional electronic and mechanical properties [1]. For instance, $MoSi_2N_4$ and WSi_2N_4 monolayers have been successfully synthesized using chemical vapor deposition, however, 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. The theoretical aspect of our work provides insights into the future nano(opto)electronic applications of MA_2Z_4 monolayers.

Structure and stability



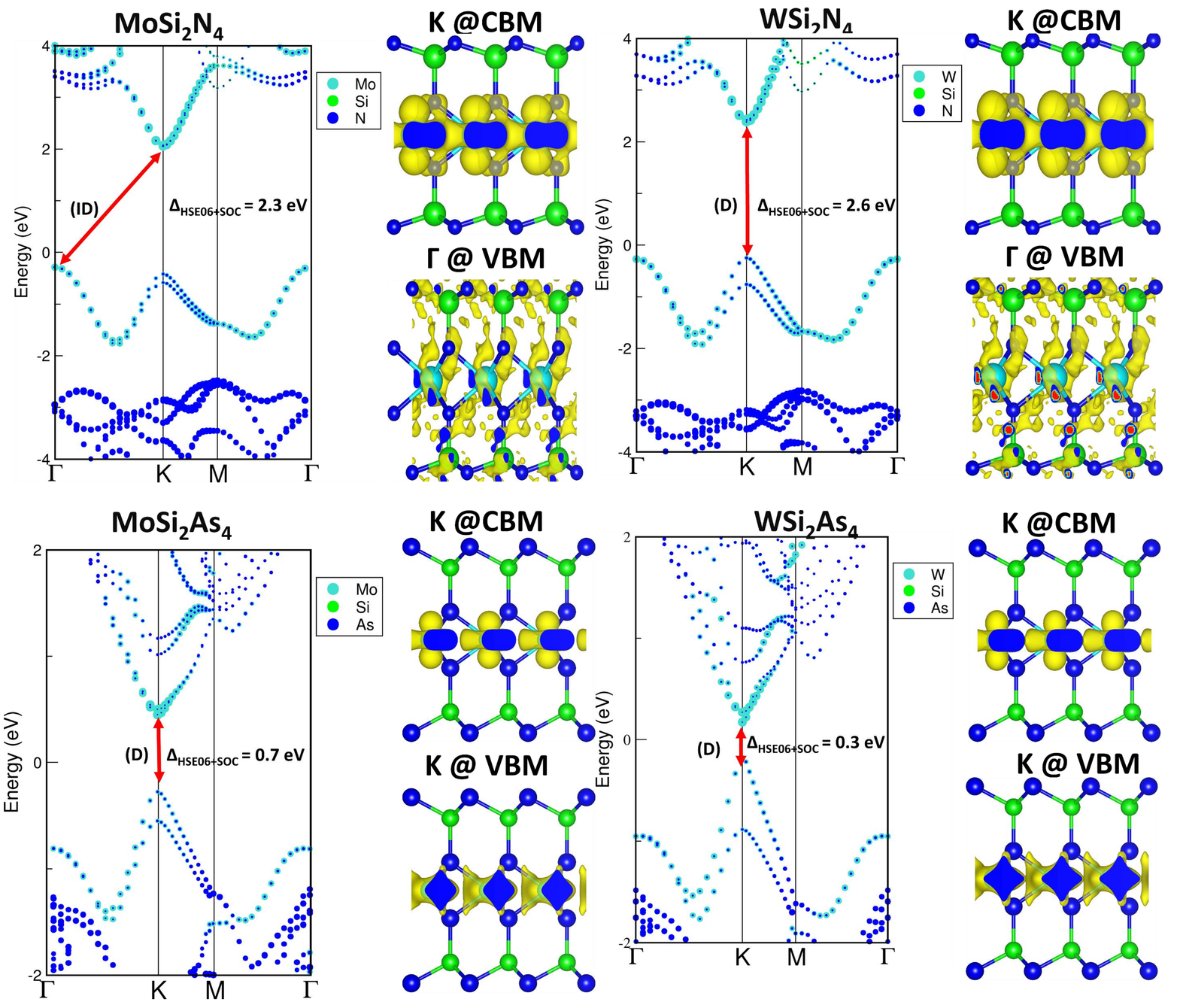
➢**All the monolayers are stable**

Properties of mixed monolayers



➢**Some of the mixtures are semiconductors whereas, others are metallic in nature**

Band structures and real-space wave function of monolayers



➢**The band gap decreases gradually by replacing the heavier element with Z**

Methods

Vienna ab initio simulation package (VASP) [3,4], DFT-D3 correction of Grimme et al.[5], Perdew-Burke-Ernzerhof (PBE)[6, 7] Heyd–Scuseria–Ernzerhof (HSE06) functional with spin orbit coupling (SOC)

Conclusion

- First principle calculations indicate that MA_2Z_4 materials possess wide tunable band gaps.
- The monolayers are in most cases direct bandgap semiconductings, except for MSi_2N_4 (indirect bandgap).
- The band gap size decreases gradually when replacing atoms with heavier elements.
- Thus, the moderate band gap and the thermodynamic stability, may pave the way for a range of applications in areas including energy, 2D electronics and optoelectronics.

CONTACT PERSON

Umm-e-Hani
u.asghar@jacobs-university.de

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.
[3] Kresse G and Hafner J, Phys. Rev. B,47 (1993): 558-61.
[4] Kresse G and Furthmuller J, Comp. Mater. Sci. 6 (1996): 15-50.
[5] Grimme S, Antony J, et al., J. Chem. Phys. 132 (2010): 154104.
[6] Perdew J P and Yue W, Phys. Rev. B 33 (1986): 8800-2.
[7] Perdew J P, Burke K and Ernzerhof M, Phys. Rev. Lett. 77 (1996): 3865-8.

chem2Dmat
AUGUST 31 - SEPTEMBER 03, 2021 • ONLINE