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Electronic and Excitonic Properties of MSi2Z4 Monolayers

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Abstract

MA_2Z_4 monolayers form a new class of hexagonal non-centrosymmetric materials hosting extraordinary spin-valley physics [1]. While only two compounds ($MoSi2N_4$ and $WSi2N_4$) were recently synthesized, theory predicts interesting (opto)electronic properties of a whole new family of such two-dimensional materials [2]. Here, the chemical trends of band gaps and spin-orbit splittings of bands in selected MSi_2Z_4 (M = Mo, W; Z = N, P, As, Sb) compounds are studied from first-principles. Effective Bethe-Salpeter-equation-based calculations reveal high exciton binding energies. The evolution of excitonic energies under an external magnetic field is predicted by providing their effective g-factors and diamagnetic coefficients, which can be directly compared to experimental values. In particular, large positive g-factors are predicted for excitons involving higher conduction bands. In view of these predictions, MSi_2Z_4 monolayers yield a new platform to study excitons and are attractive for optoelectronic devices, also in the form of heterostructures. In addition, a spin-orbit-induced bands inversion is observed in the heaviest studied compound, WSi_2Sb_4, a hallmark of its topological nature.

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

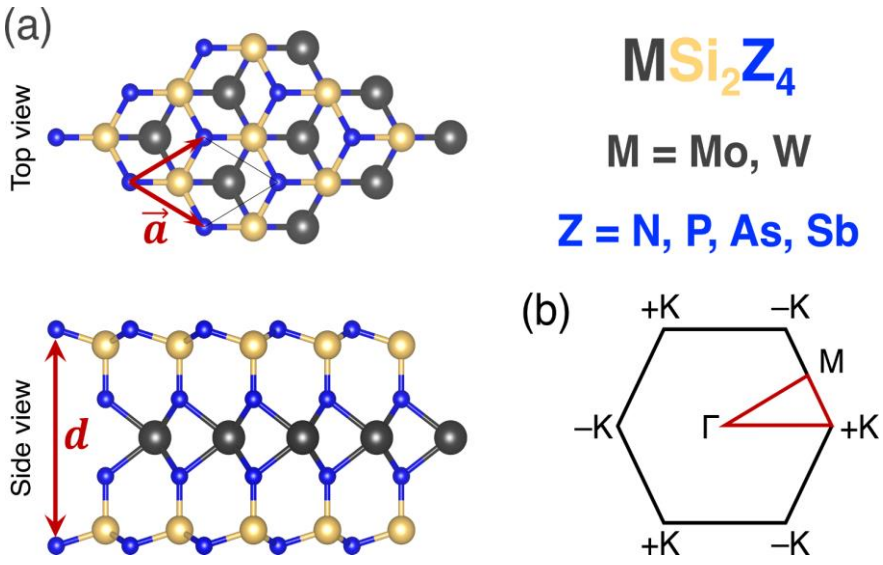

Figure 1: (a) Top and side views of 1L MSi_2Z_4 monolayer generic structure. Hexagonal unit cell is marked together with lattice vector a and the layer thickness d, defined as a distance between the outermost Z atoms. (b) The corresponding hexagonal BZ with the high-symmetry points and a path for band structure calculations (red lines).