Excellent excitonic properties of novel hexagonal MA_2Z_4 monolayers

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MA_2Z_4 monolayers form a new class of hexagonal non-centrosymmetric materials hosting extraordinary spin-valley physics. While only two compounds ($MoSi_2N_4$ and WSi_2N_4) have been synthesized so far [1], theory predicts interesting (opto)electronic properties of a whole new family of such two-dimensional materials, as analogs of transition metal dichalcogenides [2]. We study within Density Functional Theory the electronic structure of selected MSi_2Z_4 (M = Mo, W; Z = N, P, As, Sb) monolayers. They exhibit direct band gaps and significant spin-orbit splittings of bands at K valleys. Effective Bethe–Salpeter-equation-based calculations reveal exciton binding energies up to 450 meV. The wave functions of electrons and holes are confined to the inner Z-M-Z layer. Evolution of excitonic energies under 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. Additionally, a spin-orbit induced bands inversion is observed in the heaviest studied compound, WSi_2Sb_4, a hallmark of its topological nature.

In view of these predictions, MA_2Z_4 monolayers yield a new platform to study excitons and are attractive for optoelectronic devices, also as new building blocks of van der Waals heterostructures.

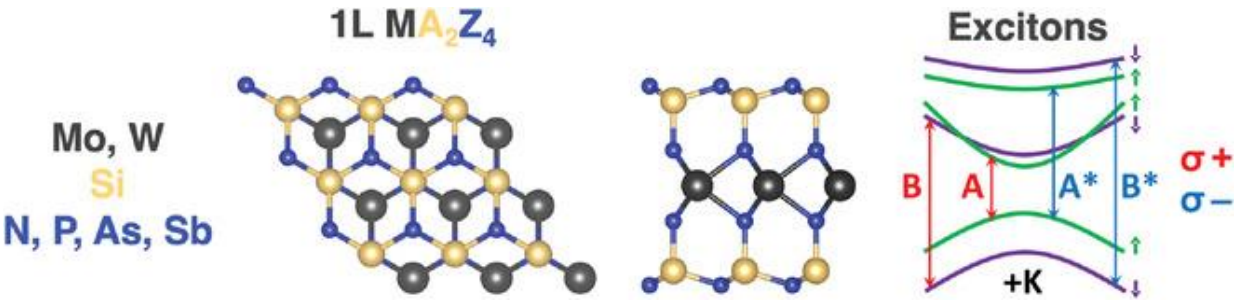

Figure 1. Top and side view of atomic structure of the studied MA_2Z_4 monolayers. Circularly polarized excitonic transitions at +K valley.

[1] Y.-L. Hong, Z. Liu, L. Wang, W. Ren et al., *Science* **369**, 670 (2021).
[2] L. Wang, Y. Shi, M. Liu, X.-Q. Chen et al., *Nature Commun.* **12**, 2361 (2021).
[3] T. Woźniak, Umm-e-hani, P.E. Faria Junior, M. S. Ramzan, A. B. Kuc, *Small*, 202206444 (2023).