Electronic structure of Ta_2NiSe_5 as a candidate for excitonic insulators

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We make the electronic structure calculations of Ta_2NiSe_5 known as a new candidate for excitonic insulators where the semiconducting or semimetallic ground state becomes unstable against the coherent formation of excitons [1,2]. We use the generalized gradient approximation (GGA) in the density functional theory, where the Hubbard-type repulsive interaction is taken into account (GGA+U). We find that the system is metallic for small values of U but an indirect band gap opens for larger values of $U \simeq 3$ eV. A flat band appears around the Γ point of the Brillouin zone but the minimum of the gap occurs away from the Γ point. Our results for the band dispersion are in contrast to the previous tight-binding bands [3] but are in reasonable agreement with recent angle-resolved photoemission spectra [1]. We discuss possible origins of observed unusual properties [1-4] of this material. Details will be reported in Ref. [5].

References:
[1] Y. Wakisaka *et al.*, Phys. Rev. Lett. **103**, 026402 (2009).
[2] F. J. DiSalvo *et al.*, J. Less-Common Met. **116**, 51 (1986).
[3] E. Canadell and M.-H. Whangbo, Inorg. Chem. **26**, 3974 (1987).
[4] S. A. Sunshine and J. A. Ibers, Inorg. Chem. **24**, 3611 (1985).
[5] T. Kaneko *et al.*, in preparation.