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**$KTi(SO_4)_2$ .$H_2O$ - a possible candidate for a new spin-Pierles system** DEEPA KASINATHAN, MPI CPfS - Dresden, Germany, GORAN NILSEN, HENRIK RONNOW, LQM-EPFL, Lausanne, Switzerland, STEFAN-LUDWIG DRECHSLER, IFW Dresden, Germnay, HELGE ROSNER, MPI CPfS, Dresden, Germnay — Recently a large number of compounds belonging to the family of $J_1$-$J_2$ chain models with competing ferromagnetic (FM) and antiferromag- netic (AFM) interactions have been discovered. In most cases, FM-$J_1$ and AFM-$J_2$ is observed, leading to helical order with no spin gap (for frustration ratio $\alpha = \frac{J_1}{J_2} \geq$ -0.25). Systems with both $J_1$ and $J_2$ being AFM causing a spin gap are rather rare. The thermodynamic data of the recently prepared $KTi(SO_4)_2.H_2O$ reveal that this system is a quasi 1D spin 1/2 chain compound with both $J_1$ and $J_2$ being AFM, and a frustration ratio $\alpha \approx 0.29$. Here we report the results of electronic structure calculations within the LSDA+$U$ method along with tight-binding models. Our calculations confirm that both $J_1$ and $J_2$ are AFM. In contrast to the experiments we obtain a larger $\alpha$, slightly depending on the choice of the Coulomb repulsion $U$ . Therefore $KTi(SO_4)_2.H_2O$ might be a new candidate for a spin-Pierles ground state. A brief comparison with other systems belonging to the class of frustrated chain materials is given with respect to their position in the general phase diagram of the 1D $J_1$ - $J_2$ model.

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