Abstract Submitted
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$Sr_2Cu(PO_4)_2$ - an unexpected one dimensional spin 1/2 Heisenberg system with isolated CuO_4 units[1] HELGE ROSNER, MPI for Chemical Physics of Solids, Dresden, MICHELLE JOHANNES, NRL Washington, JOHANNES RICHTER, Otto-von-Guericke-University Magdeburg, STEFAN-LUDWIG DRECHSLER, Leibniz Institute for Solid State and Materials Research Dresden — Recently, Belik *et. al.* [1] reported synthesis and physical properties of the compound $Sr_2Cu(PO_4)_2$. The measured magnetic susceptibility [1] exhibits a broad maximum at 92 K characteristic for quasi-1D systems, but shows no long range magnetic ordering down to 0.45 K. Here, we present full potential electronic structure calculations within the local spin density approximation, followed by a subsequent mapping to a one-band tight-binding model and an extended Heisenberg model. Although the crystal structure of $Sr_2Cu(PO_4)_2$ is formed by unlinked CuO_4 units, we find a surprisingly pronounced one dimensional behaviour with substantial coupling between nearest neighbors (NN) only. The calculated NN exchange coupling $J_1 \sim 180$ K is in good agreement with the experimental estimate. It exceeds all other couplings by at least two orders of magnitude, placing the system in the forefront of 1D spin 1/2 model compounds. Model calculations using the derived exchange constants suggest that no long range magnetic ordering should be expected down to very low temperatures.
[1]Belik *et. al.*, J. of Sol. Stat. Chem. **177**, 883 (2004).

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Helge Rosner
MPI for Chemical Physics of Solids, Dresden

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