

Abstract Submitted  
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**Ground state description of  $\text{BiCu}_2\text{PO}_6$  and  $\text{BiCu}_2\text{AsO}_6$**  DEEPA KASINATHAN, ALEXANDER TSIRLIN, OLEG JANSON, HELGE ROSNER, Max Planck Institute for Chemical Physics of Solids, Dresden — Low dimensional spin systems have always been of interest to the physics community due to their inherent exotic magnetic properties. A further impetus for the study of low-dimensional spin systems was given by the discovery of spin-ladder materials, due to the fact that they are intermediate objects between 1D and 2D systems. Recent experiments by two groups [1,2] on a spin-ladder material  $\text{BiCu}_2\text{PO}_6$  exhibited a gapped singlet ground state with a spin gap of about 34 K, though the strength of the spin-exchange interactions have remained controversial. No consensus has been reached on the correct spin-ladder model to describe this compound. We will report on our re-investigations of  $\text{BiCu}_2\text{PO}_6$  and the related material  $\text{BiCu}_2\text{AsO}_6$  using density functional theory based electronic structure calculations and as well as Transfer Matrix Renormalization Group (TMRG) calculations. Our results necessitate the inclusion of previously neglected exchange couplings to describe the spin-ladder model more adequately.

[1] B. Koteswararao, *et. al.*, Phys. Rev. B **76**, 052402 (2007).

[2] O. Mentré, *et. al.*, Phys. Rev. B **80**, 180413 (2009).

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