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Frustration in antiferromagnets and spin liquids¹

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Correlated electronic systems with an additional complexity of a geometrically frustrated lattice provide an exciting ground for the study of several competing interactions among spin, orbital and lattice degrees of freedom. In this talk we shall discuss the role of frustration in prototypical 3D-networks like the spinels ZnV_2O_4 and MnV_2O_4 and in 2D-networks like the κ -(BEDT-TTF)₂X family. By performing density functional calculations we analyze the nature of the structural, orbital and magnetic transitions in the Mott insulators ZnV_2O_4 [1] and MnV_2O_4 [2] and outline the importance of correlation effects and spin-orbit coupling on the behavior of these systems. The 2D triangular networks described by the κ -(BEDT-TTF)₂X family show a complex phase diagram with magnetic, superconducting, Mott insulating and even spin liquid phases. With extensive density functional theory calculations we refresh the link between many-body theory and experiment by determining hopping parameters of the underlying Hubbard model [3]. This leads us to revise the widely used semi-empirical parameters for these systems in the direction of less frustrated, more anisotropic triangular lattices. The implications of these results on the systems' description will be discussed and comparison to other Mott-Hubbard insulators will be shown. [1] T. Maitra and R. Valenti, Phys. Rev. Lett. **99**, 126401 (2007). [2] S. Sarkar *et al.*, Phys. Rev. Lett. **102**, 216405 (2009). [3] H. C. Kandpal *et al.*, Phys. Rev. Lett. **103**, 067007 (2009).

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