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Giant Negative Magnetization in a Class of Layered Molecular-Based Magnets¹ RANDY FISHMAN, FERNANDO REBOREDO, Oak Ridge National Lab — Bimetallic oxalates are a class of layered molecular-based magnets with transition metals M(II) and M'(III) coupled by oxalate molecules in an open honeycomb structure. Energy, structure, and symmetry considerations are used to construct a reduced Hamiltonian, including exchange and spin-orbit interactions, that explains the magnetic compensation and giant negative magnetization in some of the ferrimagnetic Fe(II)Fe(III) compounds. By shifting the Fe(II) ions with respect to the oxalate molecules, the organic cation between the magnetic layers alters the C₃-symmetric crystal field and the orbital angular momentum of the ground-state doublet at the Fe(II) sites. We provide new predictions for the spin-wave gap, the effects of uni-axial strain, and the optical flipping of the negative magnetization in Fe(II)Fe(III) bimetallic oxalates [1]. [1] R.S. Fishman and F.A. Reboredo, *Physical Review Letters* **99**, 217203 (2007).

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