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Electrically controlled g-factor and magnetism in conjugated metallorganic molecules[1] ZHI-GANG YU, SRI International — Conjugated metallorganic molecules have localized spins at the central transition-metal ions and mobile π-electrons in the surrounding ligands. Here we construct model Hamiltonians based on first-principles calculations to describe spins at the ions and π-electrons in the ligands. It is shown that the g-factor and magnetic susceptibility in such a molecule can be tuned to a great extent by an electrical voltage across one of the ligands. The underlying physics is that the voltage modifies the charge distribution of the ligand, which in turn changes the interplay of the the ion's spin-orbit coupling and the energy splitting among its d orbitals. The capability of controlling the g-factor and magnetism at the molecular level has great implications in quantum information storage and processing.

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Zhi-Gang Yu
SRI International

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