UNDERSTANDING THE STRUCTURE, CHEMICAL BONDING, AND SPECTROSCOPY OF MAGNETIC LANTHANIDE MOLECULES

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We have theoretically investigated the unconventional electronic structure, spectroscopic properties, and chemical bonding of highly magnetic molecules containing lanthanide (Ln) atoms. We are interested in the integration of different physical components into hybrid quantum Ln systems. This hybrid approach allows us to take advantage of each component's best properties thereby realizing new tools for quantum information processing, highly-correlated many-body physics, and high-precision measurements. First, we explore a class of homonuclear Ln molecules, where laser-cooled lanthanide atoms are brought and bound together via Feshbach resonances. Second, we theoretically investigate the unconventional chemical bond between magnetic Ln atoms and hydroxide molecules that is dominated by the behavior of its single-valence electron. Finally, we investigate the bonding of Ln atoms embedded into fullerene cages. Accurate information on the relevant potential energy surfaces and magnetic properties of these systems were previously unavailable.

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