Several postdoctoral positions are available immediately in the Center for Molecular Magnetic Quantum Materials (M2QM) at the University of Florida.   M2QM is a new (Aug. 1, 2018) Energy Frontier Research Center funded by the US Department of Energy. https://science.energy.gov/bes/efrc/

The Center focuses on the science for using molecule-based magnetic systems as the basis for the next generations of quantum technologies, with a program ranging from the synthesis and characterization of these emergent new materials to a systematic computational understanding of their many-body quantum behavior. M2QM will concentrate on fundamental scientific problems related to two technological challenges: 1) how to create qubits for intrinsically quantum computing, and 2) how to replace elements of traditional computers and sensors with intrinsically quantum, molecule-based, devices that are energy efficient as well as fast and adaptive. In this setting, reliable, swift, all-electron calculations of magnetically complex materials are crucial.

Up to 9 positions are available (8 are funded by the Center), three in experimental and six in computational/theoretical research. Successful candidates will work on –

**Experimental:**

(1) Synthesis and study of various molecule-based magnetic materials of transition metals and lanthanides, including oligomers formed by hydrogen-bonding or covalently-bound linkers. Experience in synthetic metal-oxo coordination chemistry and supramolecular chemistry would be preferred, as well as experience with techniques such as SQUID magnetometry and electrochemistry.

(2) NMR studies of molecular magnetic materials at low temperatures, including nonequilibrium dynamics of exotic quantum magnets. Experience in low temperature techniques and modern NMR methods is desired.

(3) Fabrication and characterization of thin films and thin-film heterostructures incorporating chemically fragile magnetic molecules into the interface regions of heterogeneous junctions comprising semiconductors and/or two-dimensional layered materials. Experience with clean room protocols and exfoliation techniques together with measurement techniques including X-ray diffraction, scanning probe microscopies, magnetotransport, magnetocapacitance, magnetization, tunneling, and Schottky barriers is desired. (This position will open in the summer 2019)

**Computational/theoretical:**

(1) Spin-dependent electron transport through magnetic molecules, molecular networks, and molecule-semiconductor interfaces using DFT-based methods. Experience with using both DFT and semiclassical methods is a plus.

(2) Development and implementation of algorithms to model adiabatic and nonadiabatic spin-phonon interactions within the framework of DFT and comparison with high precision quantum chemistry methods. Experience with DFT and/or quantum chemistry simulation of electron-phonon coupling preferred.

(3) Development of the Exciting-Plus full-potential LAPW code. This will include implementation of iterative eigenvalue solver and selected DFT functionals, testing, and validation of new techniques. Experience with FLAPW code development (e.g. ELK) is valuable.

(4) High throughput classic, semi-empirical, and first-principles calculations of magnetic molecules on surfaces and interfaces. Candidates with experience in the development and application of high-throughput DFT and atomistic materials simulations are desired. Knowledge of machine-learning is a plus.

(5) First-principles calculations of molecular magnetic systems. Extensive experience in DFT applications including Wannier and downfolding procedures, first-principles based many-body methods (GW, DMFT, high-level quantum chemistry) is desired. This is a research scientist position, and will also have 5-10% of responsibility working as a scientific coordinator.

(6) Radiation-induced defects in 2D materials. This will involve the application of DFT methods to describe the energetics, diffusion, and electronic properties of defects in 2D metals and semiconductors. This position is closely related to the Center activity in the area of computational/theoretical materials research and is funded by a separate experiment/theory project.

These positions are tenable for up to three years depending upon significant achievement and mutual interest. All postdoc and research scientists are expected to interact with other members including students in the M2QM center.

Interested, well-qualified candidates should send emails to m2qm.efrc@phys.ufl.edu as soon as possible.  Provide a full curriculum vitae (including publications) and contact information for three (3) references.  Please also indicate the position number(s) as listed that you are interested in.