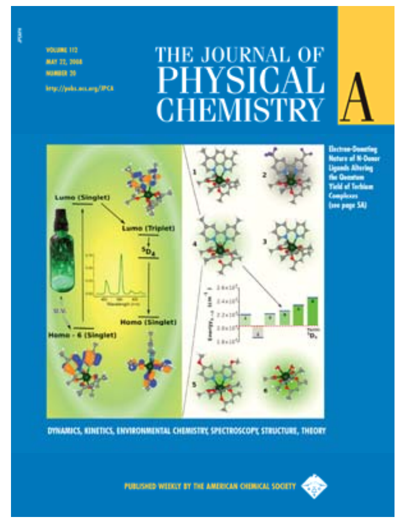
Theoreticians crack code for diodes

Study could aid in designing high-quality computer screens that use less energy

Better resolution and longer battery life are the dreams of many people using laptop computers in airports and coffee shops. Researchers want to make this dream a reality using organic light-emitting diodes, but first the diodes need new chemicals that shine brightly when exposed to an electrical current. The challenge is that scientists do not know exactly which chemicals will shine brighter than others. The key is the chemical ligands, long strings of atoms that donate and accept electrons. Designing the ligands in the laboratory is done mostly by trial and error, an expensive, time-consuming process.



This research was featured on the cover of the May 27, 2008, issue of *The Journal of Physical Chemistry A*.

So, scientists from the University of Arizona, Pacific Northwest National Laboratory, and EMSL decided to see if they could crack the code for ligand structure and composition. Using EMSL's supercomputer and the University of Arizona's computational and experimental resources, they began with experimental results on Tb(III) β-diketonate complexes, an organic molecule with a lanthanide ion at the center. This result led the way to the first time-dependent density functional theory calculations, performed on the supercomputer at the Department of Energy's EMSL. The calculations provided data on the electron acceptance and donation in ligands with different levels of current. Then, they predicted which ligands would work well in diodes. They compared these predictions to additional experimental results.

The integrated theoretical and experimental results show that the amount of light emitted by the chemical depends on the electronic properties of a specific group on the ligand, specifically the p,p'- substituent group associated with the coordinating N-donor neutral ligand. The team found that changes in the electron donating nature of the neutral ligand structure led to shifts in the energy level of the complex and consequently the amount of light produced. This information provides critical direction for the synthesis of terbium complexes that could serve to provide brighter diodes.

Scientific impact: Providing information about electron sharing on ligands involved in organic light-emitting diodes allows experimentalists to focus on the chemicals that have the greatest potential to provide the desired results. This research is one example of EMSL's effort to rapidly link theory with experiment.

Societal impact: By cutting the time needed to design chemicals for organic light-emitting diodes, this research could aid in producing computers, televisions, and other devices that consume less energy.

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