NSF-NIRT title: Nanoscale Engineering and Manufacture Effected Through Molecular Architecture and Structure

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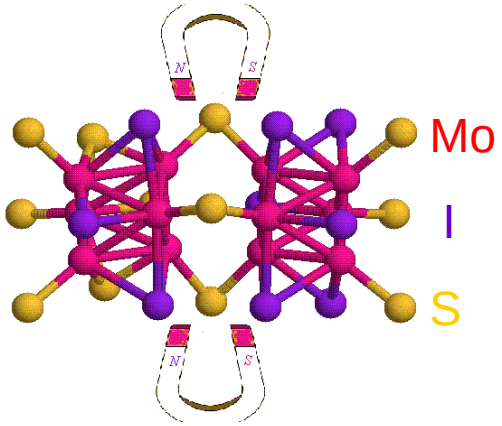
Designing functional magnetic nanowires

- **Objective:**
  - Design nanowires that memorize being stretched/compressed by switching between metallic and magnetic behavior.
- **Approach:**
  - *Ab initio* quantum chemical calculations yield equilibrium atomic positions and determine if nanowires are metallic or magnetic.
- **Significant Results:**
  - Due to their unique structure, $Mo_{12}S_9I_9$ nanowires can be reversibly stretched/compressed by up to 20% and retain their new shape.
  - This property can be utilized to construct unique mechanical strain sensors.

• Teng Yang, Shinya Okano, Savas Berber, and David Tománek, Interplay between structure and magnetism in $Mo_{12}S_9I_9$ nanowires, Phys. Rev. Lett. **96**, 125502 (2006).

Reversible magnetism in accordion-like $Mo_{12}S_9I_9$ nanowires



Charge distribution in frontier orbitals, responsible for conductivity