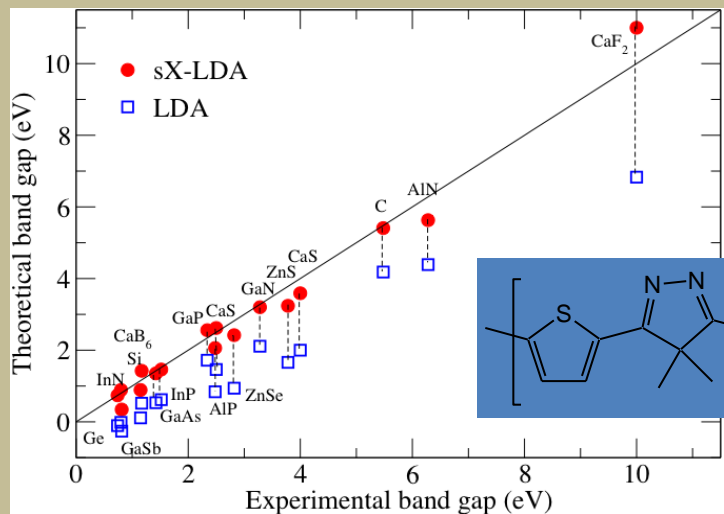


Chemistry and Physics of n-Doping Electroactive Polymers: Computationally Directed Synthesis for Improved Performance

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Problems Addressed:

- Stable n-doping polymers are needed to advance the state of the art in charge storage, LEDs, photovoltaics, and electrochromics
- n-Doping polymers are notoriously unstable; improve stability by incorporating imine-type nitrogens along the polymer backbone
- Current computational modeling approaches fall short

Status/ Approach:

GOAL: produce excellent new computational modeling capabilities and novel, stable n-doping polymers

- Use fundamental principles to design, model, synthesize, and characterize n-doping polymers based on nitrogen-containing heterocycles.
- Apply LS3DF/sX-DFT to rapidly predict electronic properties of electroactive polymers consisting of thousands of atoms.
- Evaluate electronic properties and use values to validate modeling methods.

Expected Results:

- Stable n-doping polymers
- Sophisticated computational modeling capability
- Better understanding of electronic properties
- Enhanced collaboration between Chemistry and Physics Departments

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