SD2 (Energy Materials) Annual Progress

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LA-SiGMA
Louisiana Alliance for Simulation-Guided Materials Applications

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We have Investigations in Multiple Areas with Respect to Hydrogen Storage

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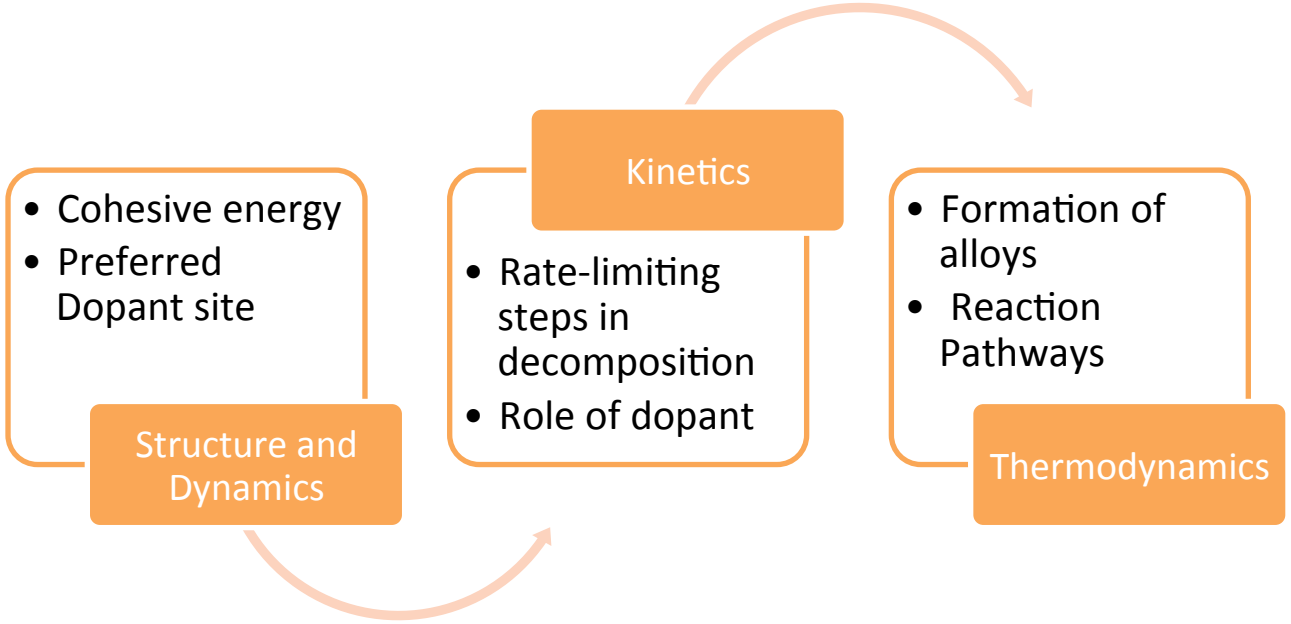
We Have Developed a Strategy for Improving Hydrogen Storage

- **SD2, F2 : Thermodynamics and Kinetics in Hydrogen Storage Systems**
- **Goal** : Improve ability to design materials for hydrogen storage/explore wide range of promising hydrogen storage systems
- **Method** : First-principles investigation of effect of catalytic additives in improving atomic mobility and desorption rates in CMHs



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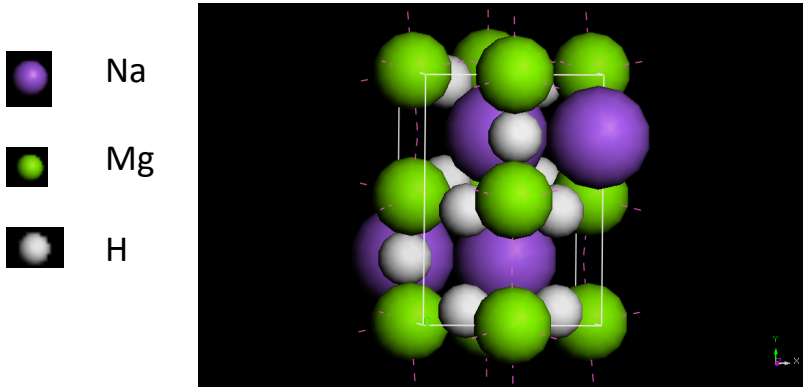
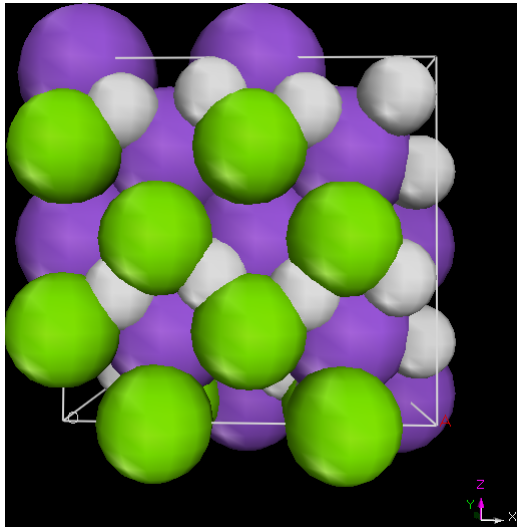
We Are Working to Improve $NaMgH_3$

- **Complex Metal Hydrides** have attracted interest, experimental findings show that decomposition temperature for CMHs can be modified by introduction of additives



- **Structure and Dynamics Stage**
  Overall goal of First Principles calculations for 3d-Transition Metal **Doping** is to determine**:**
  - Structural stability
  - Preferred doping site
  - Cohesive energy



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We Made Significant Progress in Understanding the Structure and Dynamics of Doped $NaMgH_2$ Materials

- Ti-Mg_xH_x complexes are observed after geometry optimization of doped-surface models
- DFT coupled MD simulations show the existence of Ti-Mg_xH_x,
- Substitution and addition energy of surface models show that Ti @ Hollow site and Ti @ Na lattice site have almost equal energies
- Ti @ Hollow site may act like a zipper effect and diffuse through bulk and the surface, creating Na rich and Mg rich sites
  - Further study of this include modeling with four layers slab

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We have plans for the future

- Work with Carbon, it has one of the highest cohesive energies in periodic table
- Try other dopants such as Cesium or Fluorine
- Instead of doping with just one atom, optimize the complex and use it as a dopant (single dopants act as point defects and may cause the system to be trapped in local minima)


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Band Gap 1

- We have initiated the project as planned. significant research has been accomplished. The focus was strictly to hone the Bagayoko, Zhao, and Williams method
- that predicts, from first principle, electronic and related properties of materials. In particular, our calculations of properties of wurtzite ZnO and CdS, zinc blende CdS, rutile TiO2 are the first ab-initio ones known to us to obtain the measured band gaps of these materials, respectively. The first highlight from my group is attached. It is on wurtzite ZnO (w-ZnO) for which we obtained measured electronic properties, including the band gap.*Stupendous implications of this feat, as noted in the highlight, consist of highly accurate predictive capabilities for first principle calculations to inform and to guide the design and fabrication of semiconductors and nanostructure based devices.*


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Hall Stuff

- Les Butler has images of hydrogen uptake in the material LaNi5. We are developing a force field for use with grand canonical and/or Bin Chen's aggregation volume bias - umbrella sampling Monte Carlo simulations of hydrogen uptake as a function of applied H2 pressure. The force field is an embedded atom potential along the lines of those the Emily Carter used to study hydrogen in alpha-iron. Attached are radial distribution functions showing crystal structures and 1K canonical simulations of LaNi5 and LaNi5H6 showing the quality of the current force field. Energetics associated with the force field are accurate to around .1 eV (sublimation energies, reaction energies) and bulk moduli accurate to about 1%

- Bin Chen and RWH along with LA-SiGMA REU student Igor Kolesnichenko and LA-SiGMA grad student Brandon Borill will be testing the MC methods on LaNi5H6. With the help of Daniella Mainardi and her student Francisco Soto, Brandon is beginning work on force fields for the hydrides studied by Daniella and Francisco.