LEHIGH UNIVERSITY | Institute for Functional Materials and Devices (I-FMD)

Data-Driven Design of Next-Generation Quantum Materials and Interfaces

Computational Materials Research Group

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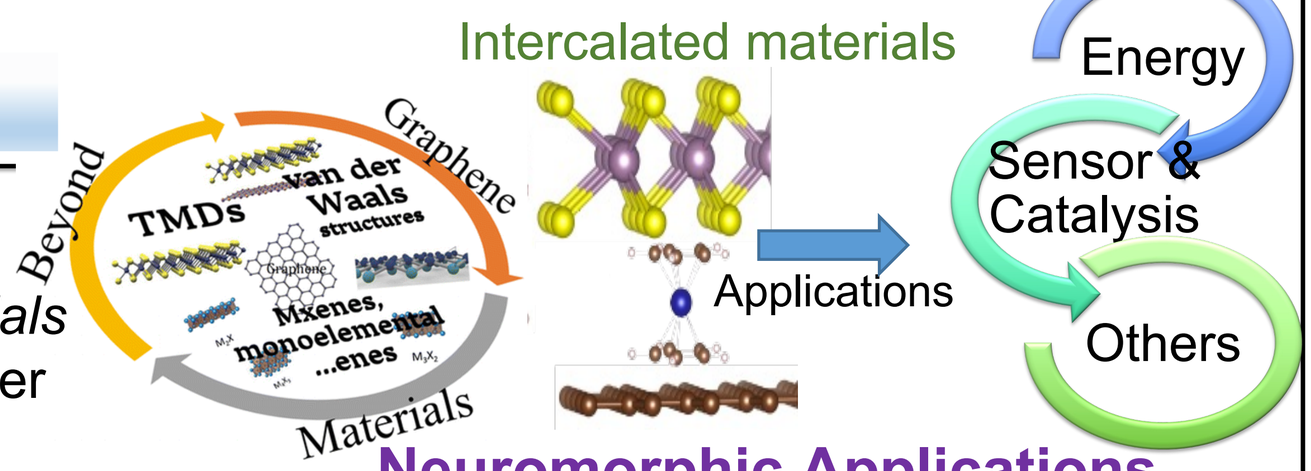
Designing for Next-generation Devices



➢ Predictive modeling

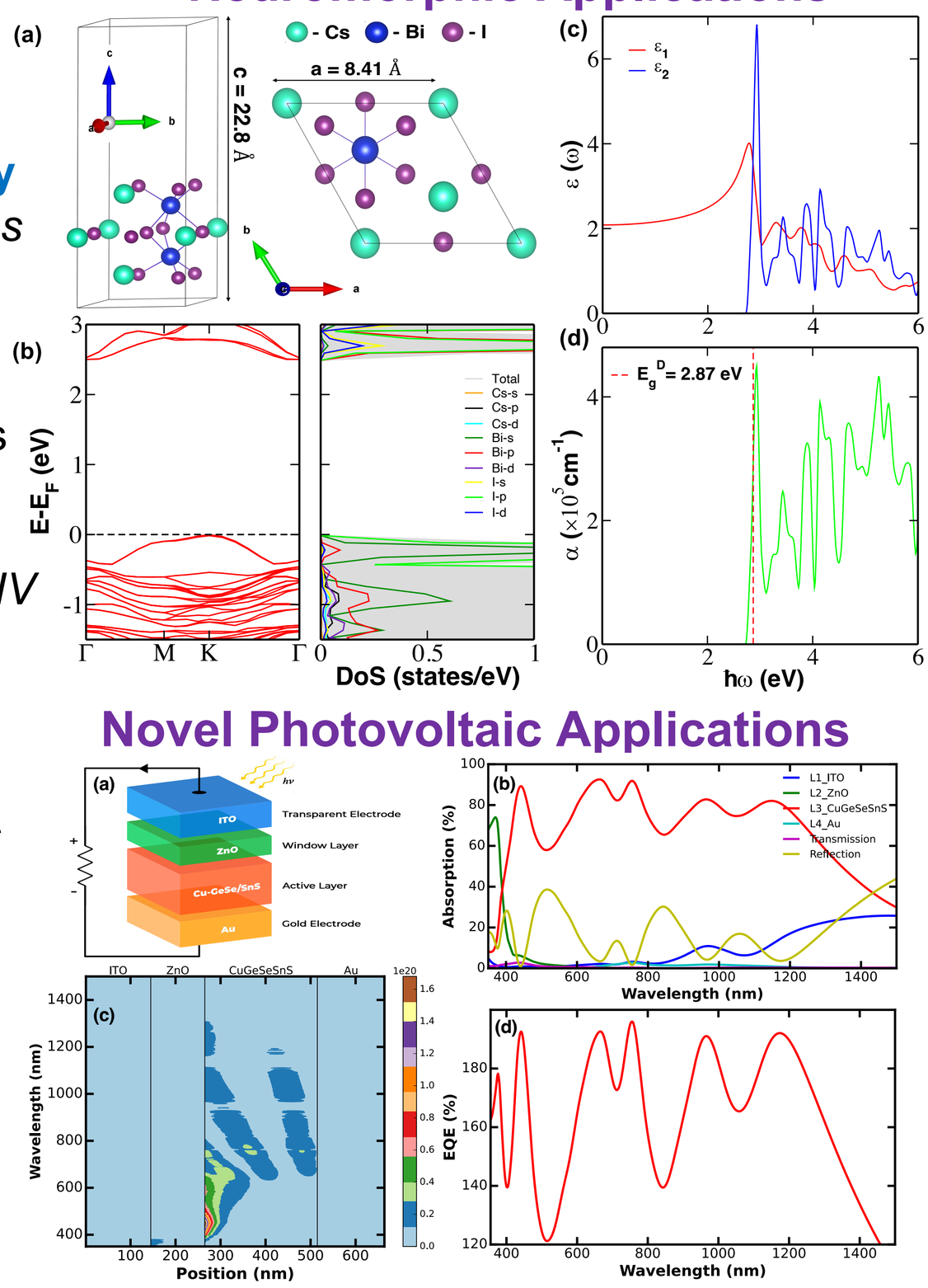
- *Novel features in atomically thin 2D materials*
- Engineering the exotic phases in 2D van der Waals and organic molecules hybrids
- Defect/strain-engineering of nontrivial phases such as MIT quantum phases in strongly correlated systems

➢ Computational materials design and discovery

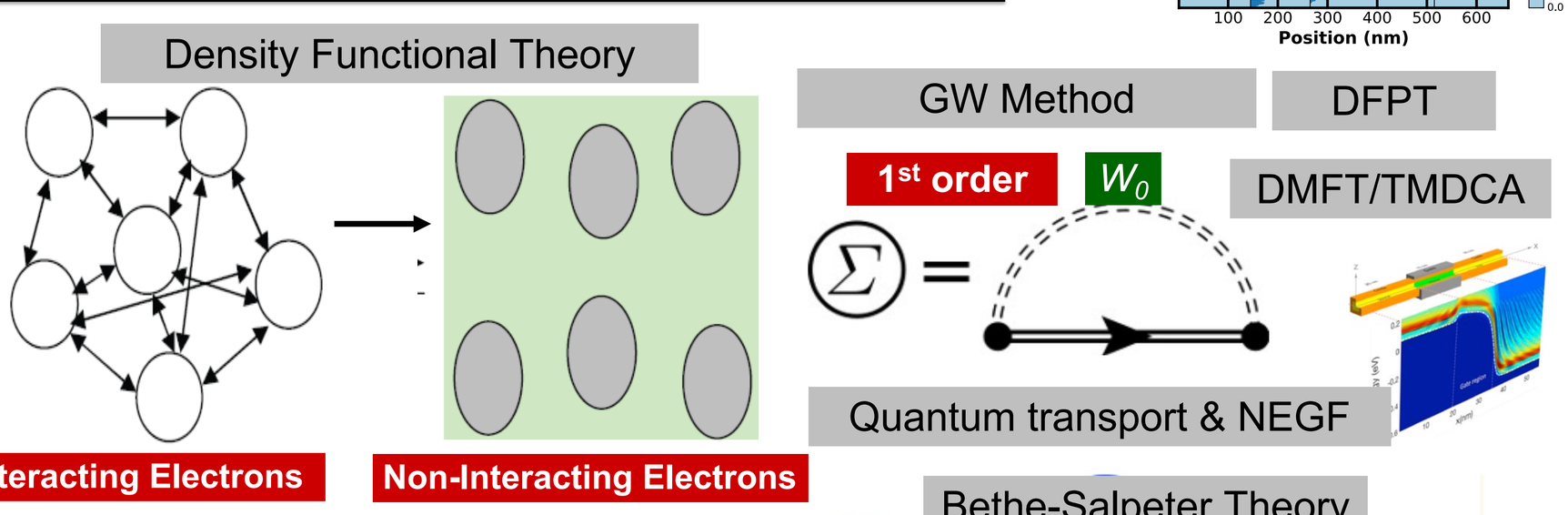
- *Inverse design and discovery of target properties*
- *New advanced materials discovery*
- *Computational guided experimental synthesis*
- Computational framework assisted active machine learning and data-driven new materials discovery

➢ Device Simulations

- *Engineering ultrafast carrier dynamics in group-IV monochalcogenides through zerovalent functionalization*
- *Design and discovery of intermediate band semiconductor with quantum efficiency beyond the Shockley–Queisser limit for novel solar cells*
- *Spin-filter MTJ with giant TMR ratio using ferrimagnetic electrodes for spintronics applications*
- *Design and discovery of all-inorganic lead-free 2D perovskites with giant electrophotonic response*



Diversity of Computational Techniques



References:

1. Liu, Z.L. *et al.* "ElasTool: an automated toolkit for elastic constants calculation." *Computer Physics Communications,* **270** (2022): 108180.
2. Kastuar, S. M. *et al.* "Efficient prediction of temperature-dependent elastic and mechanical properties of 2D materials." *Scientific Reports* **12** (2022): 3776.
3. Kastuar, S.M. *et al.* "Giant electrophotonic response in two-dimensional halide perovskite $Cs_3Bi_2I_9$ by strain engineering." *Phys. Rev. Mat.* **7** (2023): 024002.
4. Kastuar, S. M., *et al.* "Giant intrinsic magnetoresistance in spin-filtered tunnel junctions with ferrimagnetic electrode." *Phys. Rev. B* **107** (2023): 155305.

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