UNL Department of Physics and Astronomy presents:

Designing Functional Materials One Atom at a Time

PRESENTED BY

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THURSDAY

APRIL 27

4:00 PM

IN JH 136

Refreshments will be served in the JH 1st Floor Vending Area at 3:30

ABSTRACT

Defects in materials are inevitable. Sir Colin Humphreys wrote "crystalsare like people, it is the defects in them which tend to make them interesting".[1] Advances in supercomputing capabilities and

first-principles calculations based on density-functional theory now make it possible to successfully describe the properties of "real"

materials with disorder, defects, and imperfections starting from the atomic scale. Concurrent advances in scanning transmission electron

microscopy enable imaging and spectroscopy of the atomic and

electronic structure of materials with unprecedent spatial and energy resolution. Naturally then, the combination of theory and microscopy provides an unparalleled probe to unravel the structure-property

correlations in real materials. In this presentation, I will discuss my group's efforts to develop new materials with defects and disorder for energy and optical applications. Examples will include design of

defective oxides for cleaner combustion of hydrocarbons,[2]

two-dimensional high-entropy alloys for CO_2 reduction,[3,4] and

chalcogenide perovskites with colossal optical anisotropy.[5]

1. C. J. Humphreys, in *Introduction to Analytical Electron Microscopy*, (Eds: J. J. Hren, J. I. Goldstein, D. C. Joy), Springer US, Boston, MA 1979, 305.
2. G. F. Luo *et al.*, J. Phys. Chem. C **123**, 17644 (2019).
3. J. Cavin *et al.*, Adv. Mater. **33,** 2100347 (2021).
4. Z. Hemmat *et al.*, Adv. Mater. **32,** 1907041 (2020).
5. H. Mei *et al.*, arXiv:2303.00041 (2023).