2-D Materials:
A New Frontier in Energy Storage and Electronics

Nano Utah 2015

Casey Hawkins

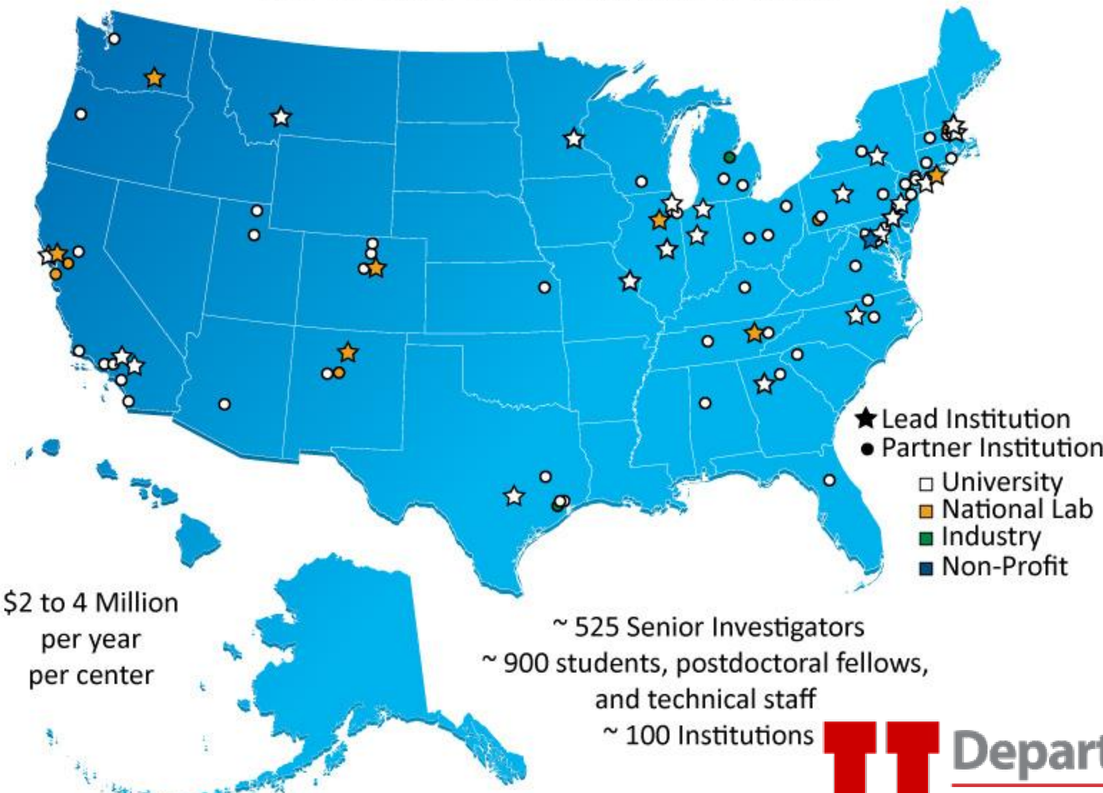
13 October 2015

Department of Chemistry
COLLEGE OF SCIENCE | THE UNIVERSITY OF UTAH

Energy Frontier Research Center

- **integrated, multi-investigator Centers** involve partnerships among universities, national laboratories, nonprofit organizations, and for-profit firms that will conduct fundamental research
- Transforming the way we **generate**, **supply**, **transmit**, **store**, and **use** energy will be one of the defining challenges for America and the globe in the 21st century.
- Competed 4-5 yr Awards to address **Grand Challenges**

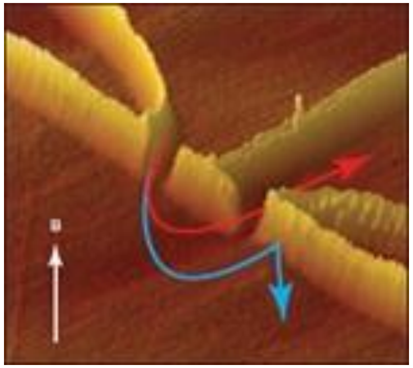
32 EFRCs in 33 States + D.C.



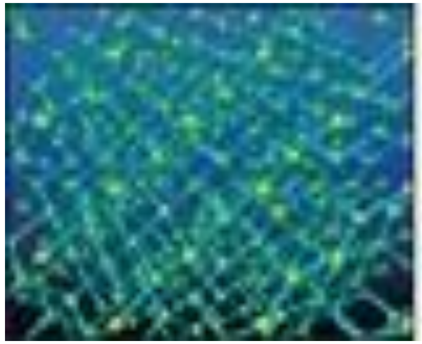
Department of Chemistry
COLLEGE OF SCIENCE | THE UNIVERSITY OF UTAH

http://science.energy.gov/bes/efrc/research/grand-challenges/

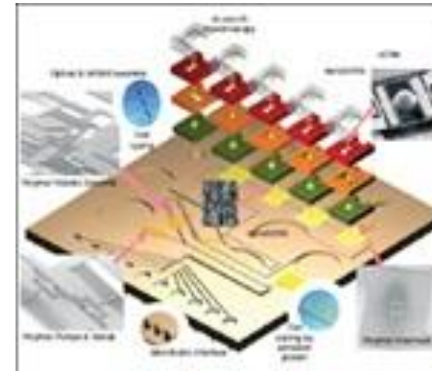
Grand Challenges



How do we **control** materials processes at the level of **electrons**?



How do remarkable properties of matter emerge from **complex correlations of the atomic or electronic constituents** and how can we control these properties?



How can we **master energy and information on the nanoscale** to create new technologies with capabilities **rivaling those of living things**?

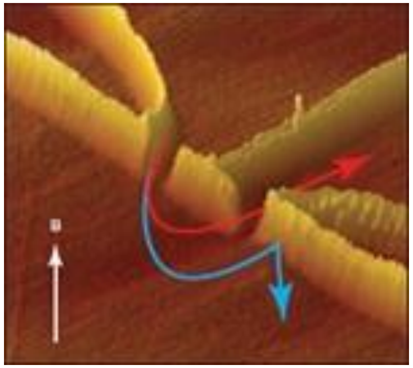
How do we **design revolutionary new forms of matter** with tailored properties?

How do we characterize and control matter **away - especially very far away - from equilibrium**?

Department of Chemistry
COLLEGE OF SCIENCE | THE UNIVERSITY OF UTAH

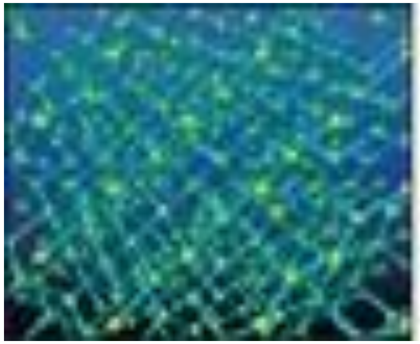
http://science.energy.gov/bes/efrc/research/grand-challenges/

Grand Challenges



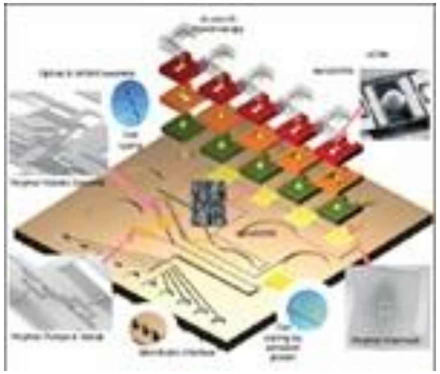
How do we **control** materials processes at the level of **electrons**?

How do we **design revolutionary new forms of matter** with tailored properties?



How do remarkable properties of matter emerge from **complex correlations of the atomic or electronic constituents** and how can we control these properties?

How do we characterize and control matter **away - especially very far away - from equilibrium**?



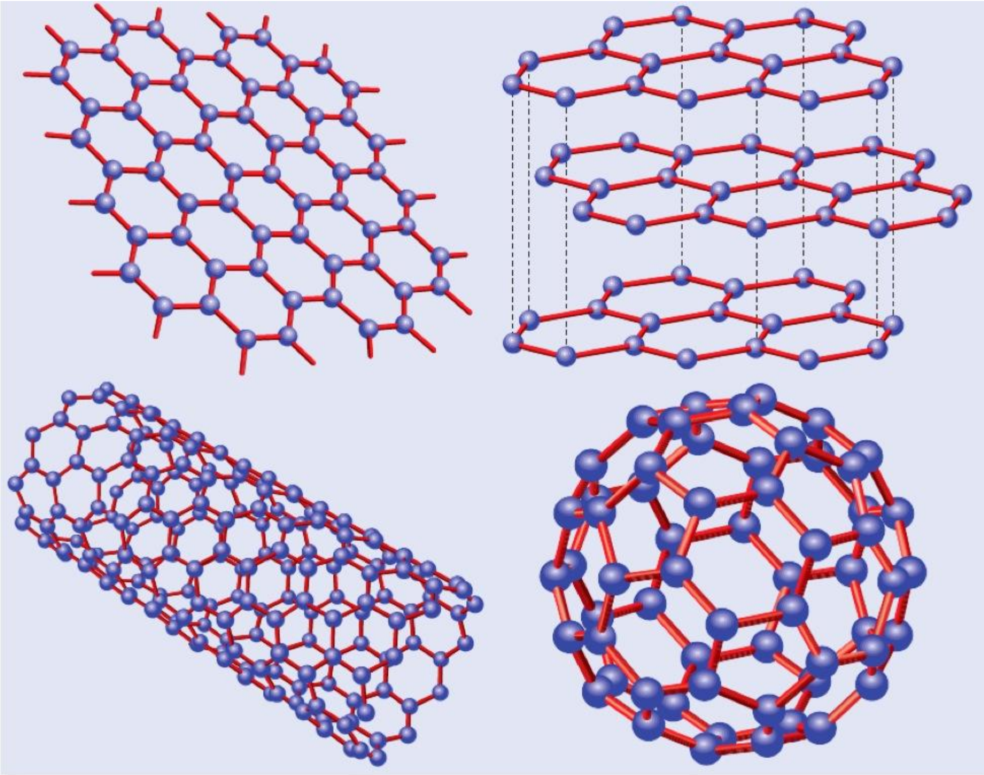
How can we **master energy and information on the nanoscale** to create new technologies with capabilities **rivaling those of living things**?

Department of Chemistry
COLLEGE OF SCIENCE | THE UNIVERSITY OF UTAH

http://science.energy.gov/bes/efrc/research/grand-challenges/

2-D Materials

- Extended 2-D structure

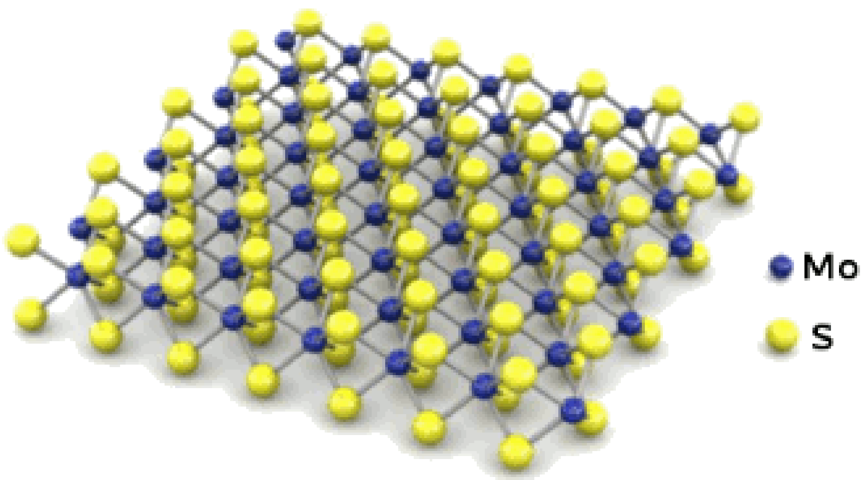


http://graphene.nus.edu.sg/content/graphene

Department of Chemistry
COLLEGE OF SCIENCE | THE UNIVERSITY OF UTAH

2-D Materials

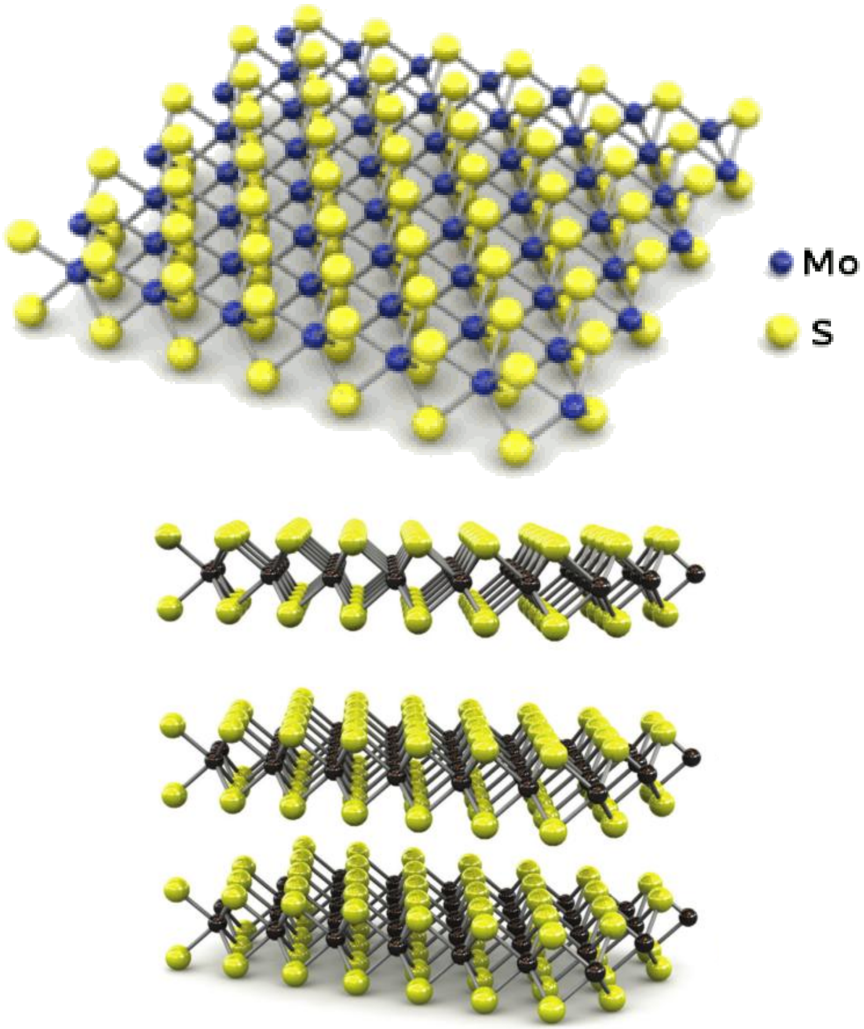
- Extended 2-D structure



http://tikalon.com/blog/blog.php?article=2011/MoS2
Radisavljevic, B., Radenovic, A., Brivio, J., Giacometti, V. & Kis, A. Single-layer MoS_2 transistors. (2011). doi:10.1038/NNANO.2010.279

2-D Materials

- Extended 2-D structure
- Weak out-of-plane van der Waals interactions
- Can be cleaved from 3-D bulk material



http://tikalon.com/blog/blog.php?article=2011/MoS2
Radisavljevic, B., Radenovic, A., Brivio, J., Giacometti, V. & Kis, A. Single-layer MoS_2 transistors. (2011). doi:10.1038/NNANO.2010.279

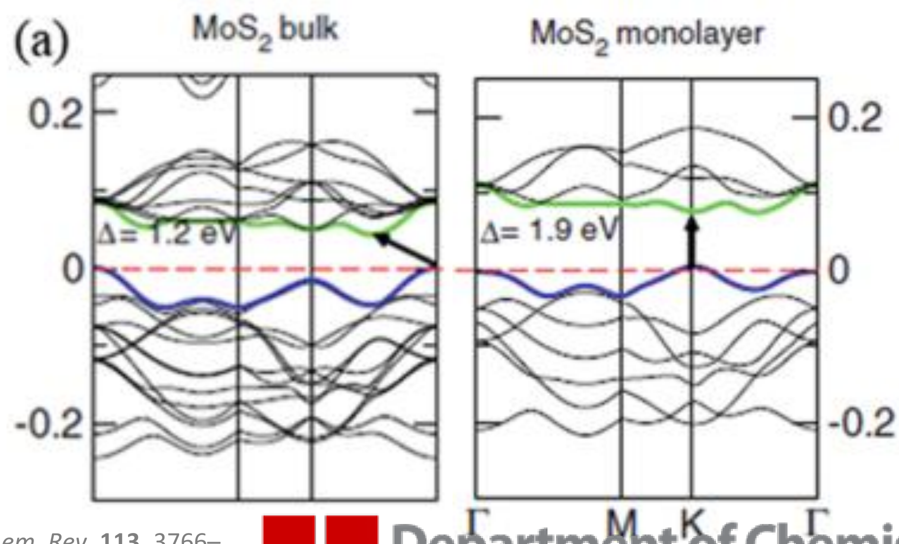
Department of Chemistry
COLLEGE OF SCIENCE | THE UNIVERSITY OF UTAH

2-D Materials

- Extended 2-D structure
- Weak out-of-plane van der Waals interactions
- Can be cleaved from 3-D bulk material
- Lamellar structure allows for tuning of electronic properties
- Unique electrical, mechanical, and chemical properties

Table 1. Summary of the Band Gaps of Typical Layered TMDs and *h*-BN Materials

2D sheets	theoretical E_g (eV)	experimental E_g (eV)
graphene	0	0
bilayer graphene	0	0
bulk *h*-BN		5.97 [ref 52]
monolayer *h*-BN		6.07 [ref 65]
fully hydrogenized *h*-BN	3.05 [ref 66]	
2–5 layers *h*-BN		5.92 [ref 105.]
bulk MoS_2	1.20 (indirect[b]) [refs 35, 139]	1.0–1.29 (indirect) [refs 35, 139]
monolayer MoS_2[a]	~1.90 (direct[b]) [ref 140]	~1.90 (direct) [ref 140]
bulk WS_2	~1.30 (indirect[b]) [refs 35, 147]	~1.35 (indirect) [refs 35, 147]

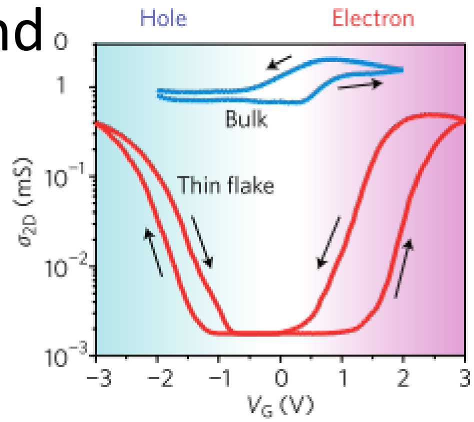


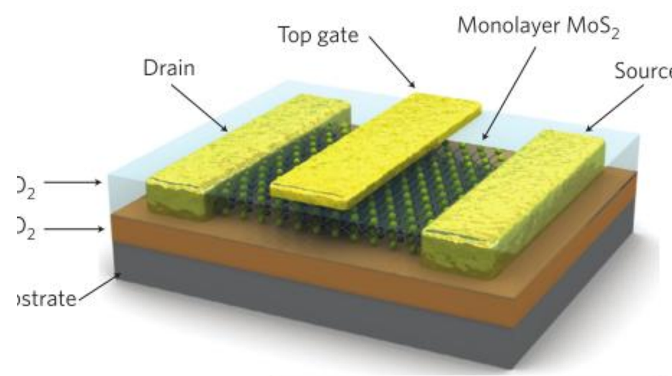
Xu, M., Liang, T., Shi, M. & Chen, H. Graphene-like two-dimensional materials. *Chem. Rev.* **113,** 3766–3798 (2013)
Radisavljevic, B., Radenovic, A., Brivio, J., Giacometti, V. & Kis, A. Single-layer MoS_2 transistors. (2011). doi:10.1038/NNANO.2010.279

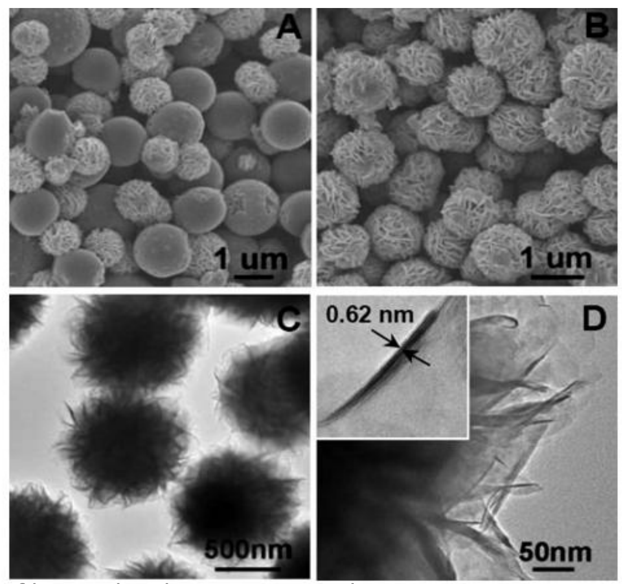
Department of Chemistry
COLLEGE OF SCIENCE | THE UNIVERSITY OF UTAH

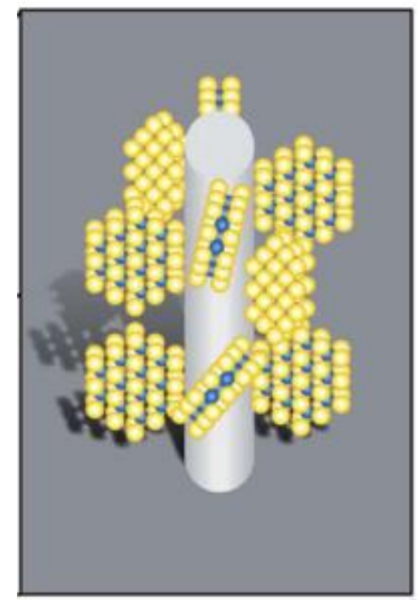
2-D Material Application

- 2-D materials have found applications in:
  - Optoelectronics
  - Spintronics
  - Catalysts
  - Chemical and biological sensors
  - Supercapacitors
  - Solar cells
  - Field-effect Transistors
  - Lithium ion batteries



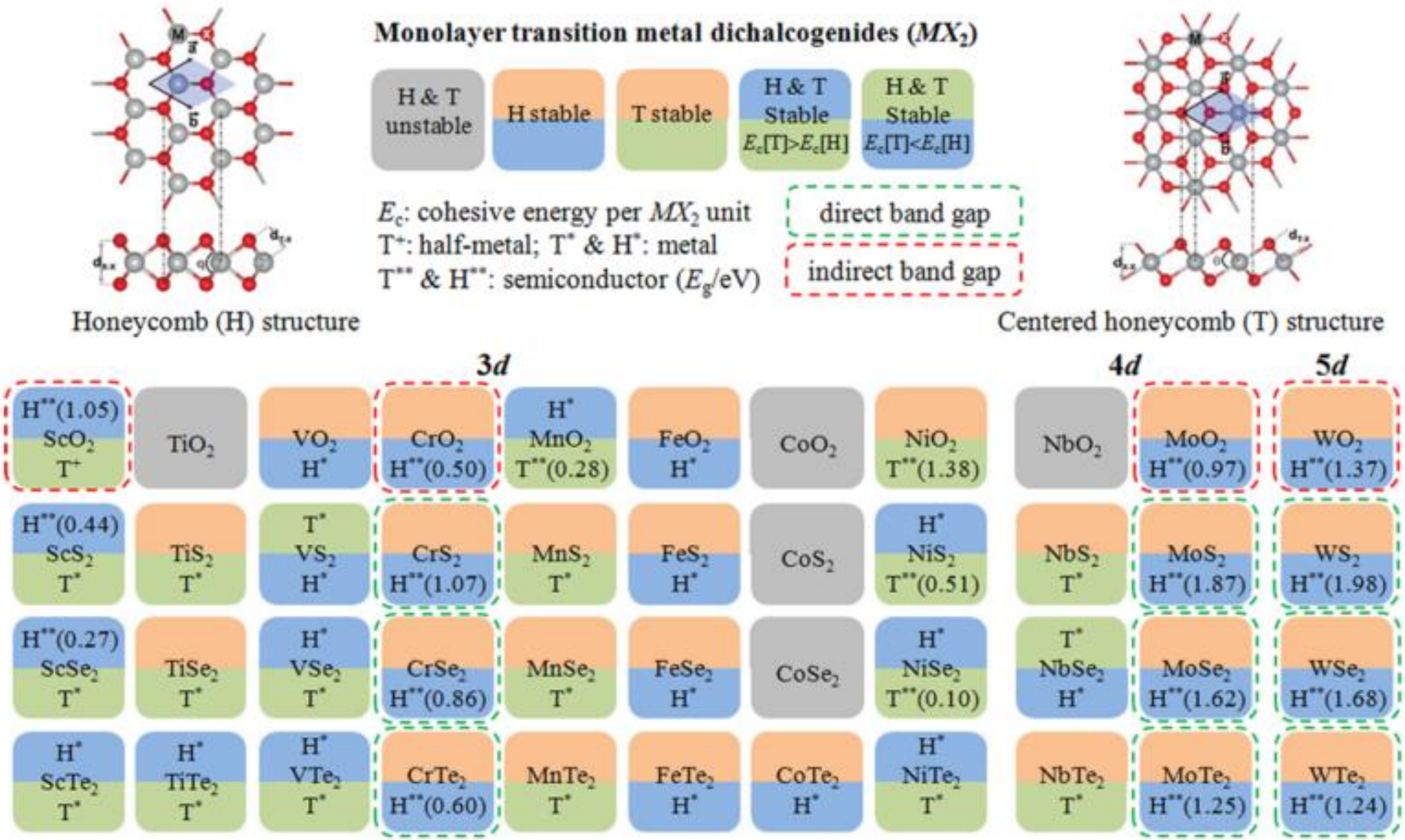






Ding, S., Zhang, D., Chen, J. S. & Lou, X. W. (David). Facile synthesis of hierarchical MoS_2 microspheres composed of few-layered nanosheets and their lithium storage properties. *Nanoscale* **4,** 95–98 (2012).
Laursen, A. B., Kegnæs, S., Dahl, S. & Chorkendorff, I. Molybdenum sulfides—efficient and viable materials for electro - and photoelectrocatalytic hydrogen evolution. *Energy Environ. Sci.* **5,** 5577 (201
Radisavljevic, B., Radenovic, A., Brivio, J., Giacometti, V. & Kis, A. Single-layer MoS_2 transistors. (2011). doi:10.1038/NNANO.2010.279

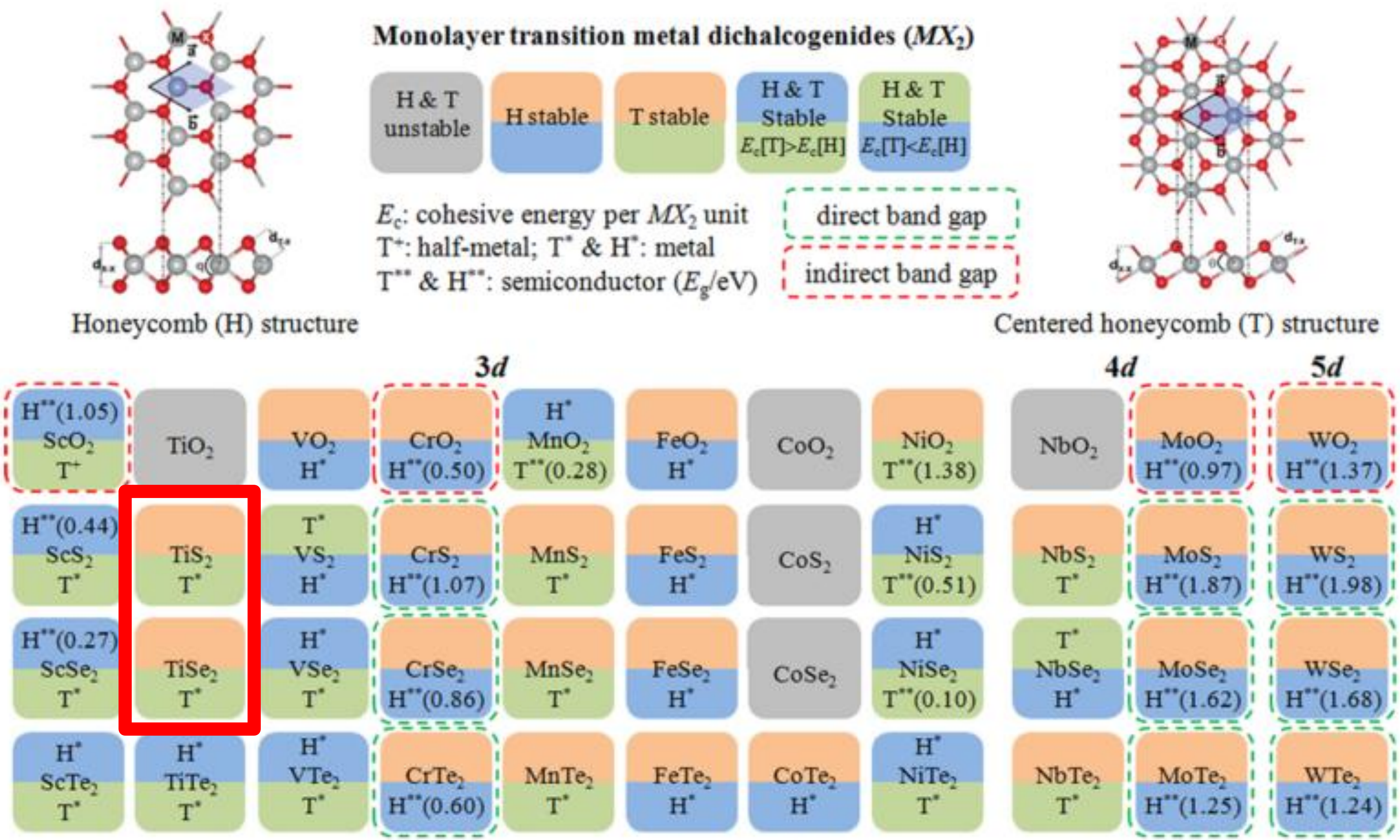
2-D Transition Metal Dichalcogenides (TMD)



Department of Chemistry
COLLEGE OF SCIENCE | THE UNIVERSITY OF UTAH

Xu, M., Liang, T., Shi, M. & Chen, H. Graphene-like two-dimensional materials. *Chem. Rev.* **113,** 3766–3798 (2013).

2-D Transition Metal Dichalcogenides (TMD)

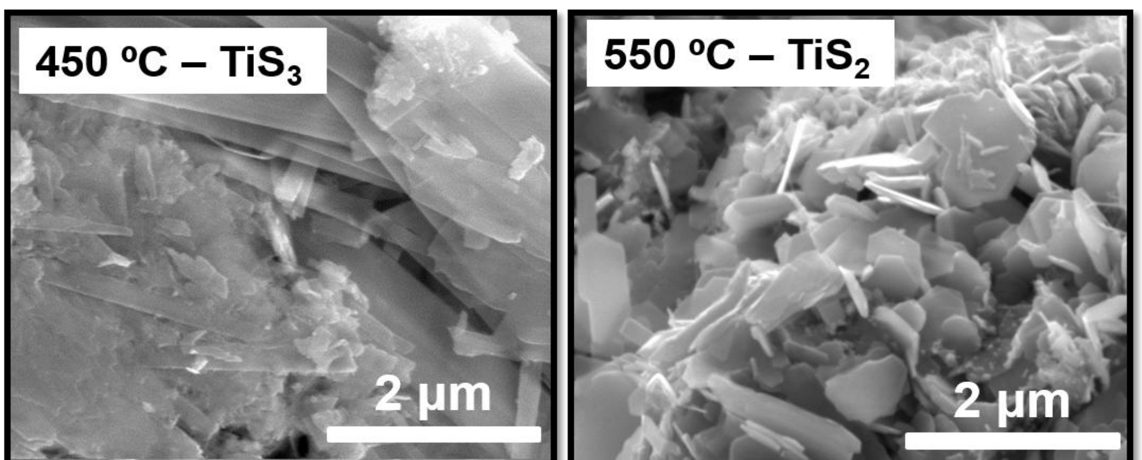


Department of Chemistry
COLLEGE OF SCIENCE | THE UNIVERSITY OF UTAH

Xu, M., Liang, T., Shi, M. & Chen, H. Graphene-like two-dimensional materials. *Chem. Rev.* **113,** 3766–3798 (2013).

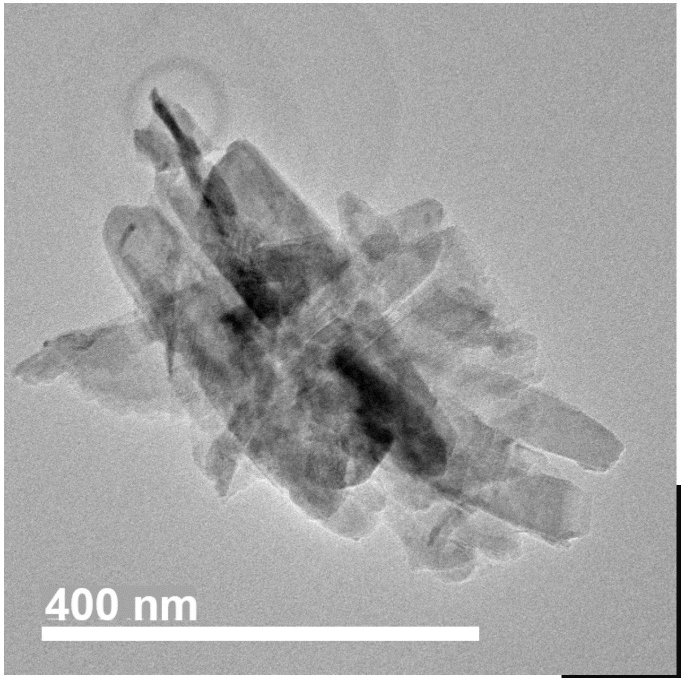
TiS_2 and TiS_3 TMD Synthesis

- Challenging to synthesize large scale mono- to few-layered systems
  - Thin film synthesis
  - Electrochemical synthesis
  - Solid-state synthesis
    - $Ti_{(s)} + 2S_{(s)} \xrightarrow[\text{ampule, 550°C}]{\text{Vacuum sealed}} TiS_{2\,(s)}$
    - $Ti_{(s)} + 3S_{(s)} \xrightarrow[\text{ampule, 450°C}]{\text{Vacuum sealed}} TiS_{3\,(s)}$



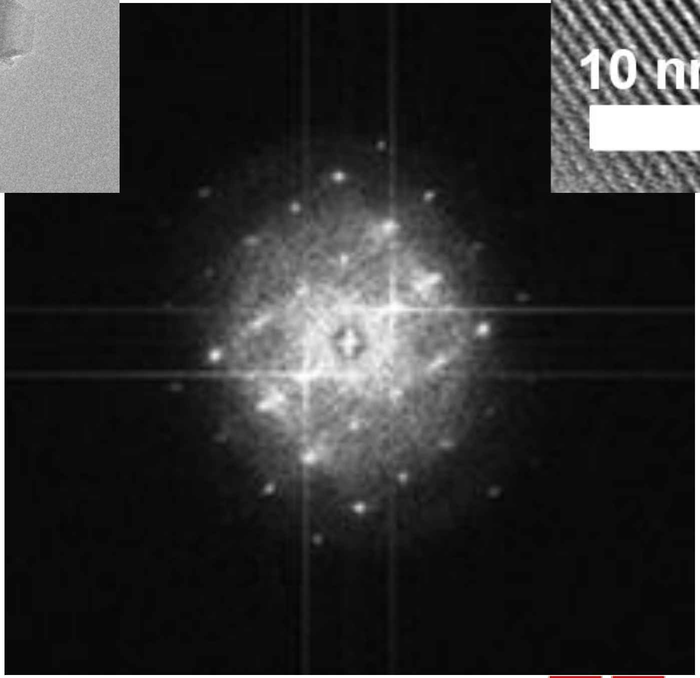
Department of Chemistry
COLLEGE OF SCIENCE | THE UNIVERSITY OF UTAH

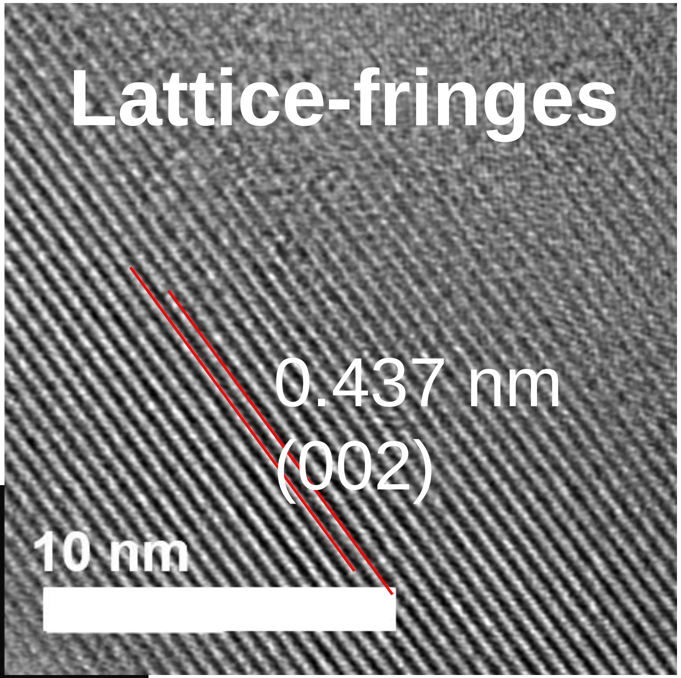
TiS_2 and TiS_3 TMD Structural Analysis



TEM

SAED



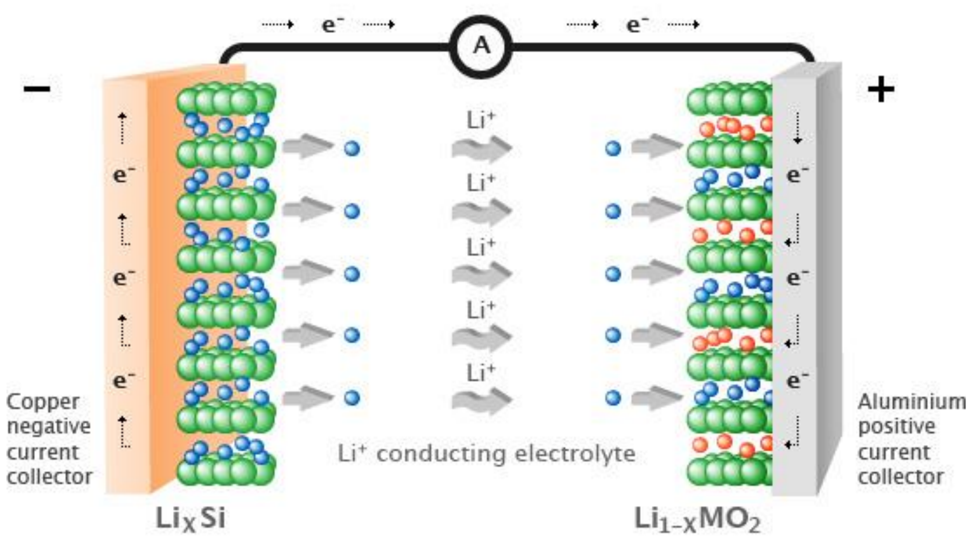


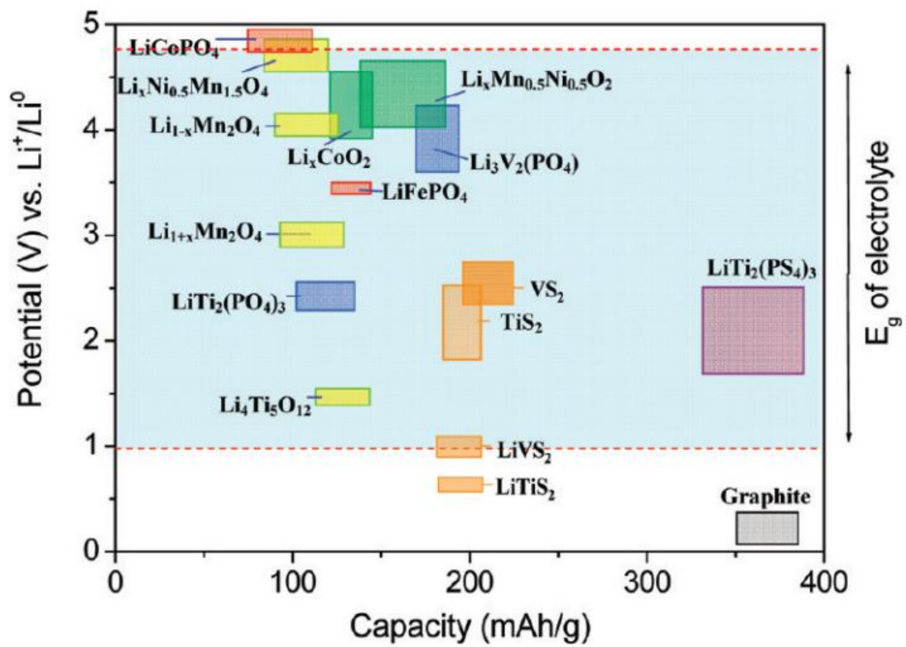
HRTEM

Department of Chemistry
COLLEGE OF SCIENCE | THE UNIVERSITY OF UTAH

Way Ahead

- Perform complete electronic property workup on TiS_2 and TiS_3
- Incorporate TiS_2 and TiS_3 into Lithium ion batteries
- Explore the electrical properties from mono-layer to bulk
- Explore the effects of dopants on the electrical properties of these systems



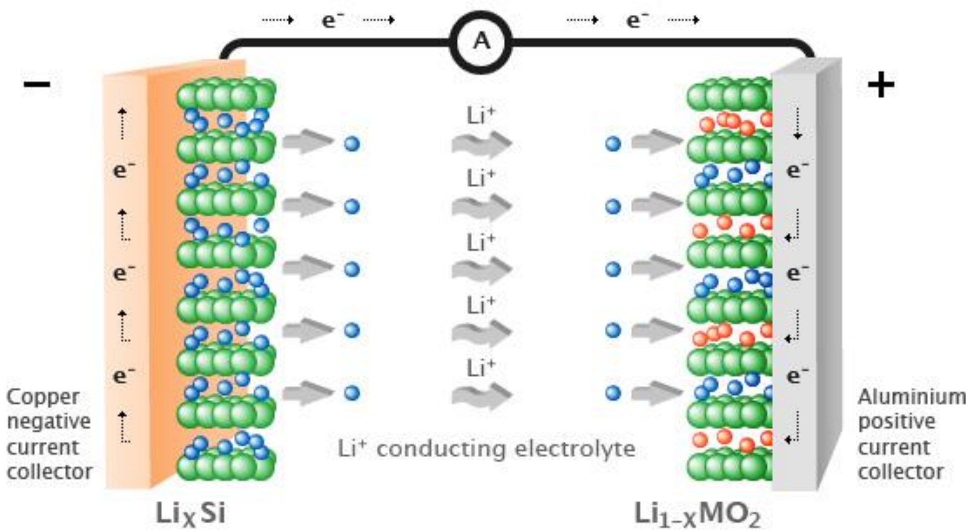


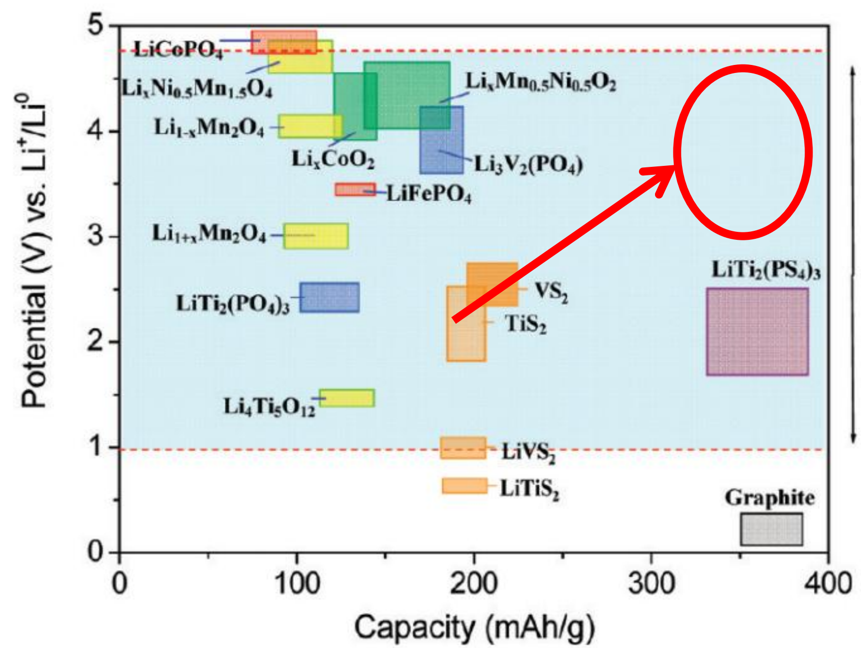
Department of Chemistry
COLLEGE OF SCIENCE | THE UNIVERSITY OF UTAH

http://www.bme.iupui.edu/~yk35/img/res-anca.png
http://nexeon.co.uk/wp-content/uploads/2009/11/test1.jpg

Way Ahead

- Perform complete electronic property workup on TiS_2 and TiS_3
- Incorporate TiS_2 and TiS_3 into Lithium ion batteries
- Explore the electrical properties from mono-layer to bulk
- Explore the effects of dopants on the electrical properties of these systems





http://www.bme.iupui.edu/~yk35/img/res-anca.png
http://nexeon.co.uk/wp-content/uploads/2009/11/test1.jpg

Department of Chemistry
COLLEGE OF SCIENCE | THE UNIVERSITY OF UTAH

Way Ahead

- Perform complete electronic property workup on TiS_2 and TiS_3
- Incorporate TiS_2 and TiS_3 into Lithium ion batteries
- Explore the electrical properties from mono-layer to bulk
- Explore the effects of dopants on the electrical properties of these systems

There is research occurring at the University of Utah that is in line with the goals and objectives of the Frontier Energy Research Center's Mission

Department of Chemistry
COLLEGE OF SCIENCE | THE UNIVERSITY OF UTAH

Questions?