Fall 2015 Joint Colloquium
Materials Department & Materials Research Laboratory

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Friday, October 30th, 2015
11:00 am, ESB 1001

Pizza served afterwards.

Emergent Phase Change and Electromechanical Properties of Two-Dimensional and Few-Layer Materials

Numerous engineering feats are being performed with the increasing array of single-layer and few-layer materials. Some of the most dramatic accomplishments are enabled by properties that emerge only at the single or few-layer limit and are not found in bulk forms. I will discuss our efforts to elucidate several new and useful emergent properties of monolayer and few-layer materials. Using and developing a variety of atomistic modeling methods, we have predicted that many of the commonly studied single-layer and few-layer transition metal dichalcogenide (TMD) materials (e.g. MoS_2) exhibit substantive electromechanical coupling in the form of piezoelectric and flexoelectric-like effects, unlike their bulk parent crystals.[1] I will describe the first recent observations of some of these effects in the laboratory by a number of research groups.

Single-layers of two-dimensional Mo- and W-dichalcogenide compounds differ from graphene in an important respect: they can potentially exist in more than one crystal structure. Some of these monolayers exhibit evidence of a structural metal-to-semiconductor transition with the possibility of long metastable lifetimes. If controllable, such a transition could bring an exciting new application space to monolayer materials. By developing electronic structure-based computational approaches, we have discovered that mechanical deformations,[2] electrostatic gating, and temperature changes all independently have the potential to control phase changes in some specific 2D materials and their alloys.[2] We further demonstrate that 2D material alloys can enable tuning of the phase boundaries over many hundreds of degrees in some cases. I will elucidate the essential aspects of thermodynamic constraints for 2D materials and contrast with those of 3D materials, and discuss the role of kinetics in the growth of 2D material alloys. The potential application space for this work ranges from information and energy storage to electronic and optical electronic devices.

References

1. Karel-Alexander N. Duerloo, Mitchell T. Ong, and Evan J. Reed, Journal of Physical Chemistry Letters **3** (19), 2871 (2012); Karel-Alexander N. Duerloo and Evan J. Reed, Nano Letters **13** (4), 1681 (2013).
2. K.-A. Duerloo, Y. Li, and E. J. Reed, Nature Communications **5**, 4214 (2014).

http://www.stanford.edu/group/evanreed/index.html

Hosted by: Michael Chabinyc