➢ Two-dimensional structural phase transitions in two-dimensional atomic materials beyond graphene (T, Barraza-Lopez)

Two dimensional atomic materials are mostly surface, such that their properties can be readily tuned by electromagnetic fields as well as mechanical strain. Barraza-Lopez's group is at the forefront of a novel aspect of these materials; namely, the possibility for some of them to undergo two-dimensional structural phase transitions [SBL1,SBL2,SBL3]. Undergraduates are early on made aware of the effects of dimensionality on physical laws, and the two-dimensional materials studied here display the effects of dimensionality in almost all their physical properties. Work in his team combines large-scale computation and basic quantum mechanics, elasticity, and chemical theory, which gives undergraduates an opportunity to explore their computational and/or theoretical abilities, while at the same time contributing to the science being produced: indeed, two undergraduates have contributed to these developments [SBL1,SBL4], and one of them was a REU student funded by this grant (Alex M. Dorio, 2014 [SBL1]). In what follows, one project with possible undergraduate involvement is delineated.

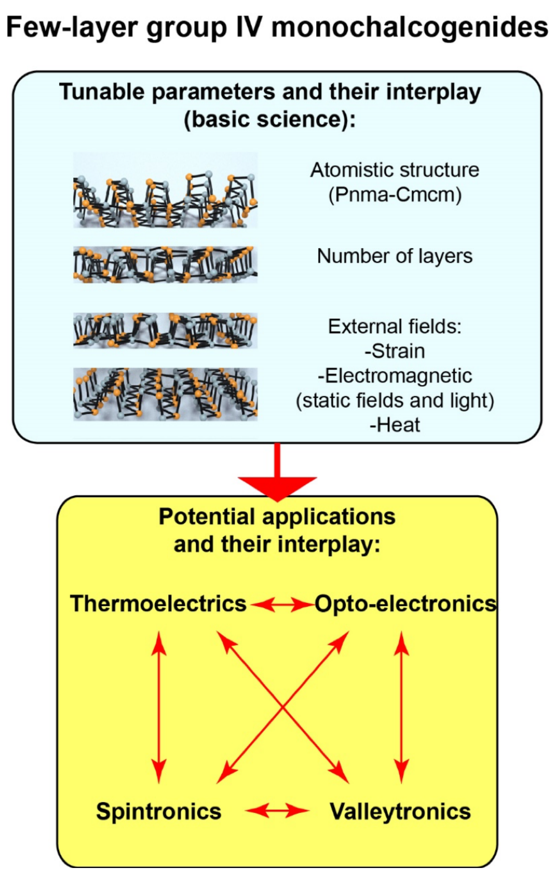

Figure 1. Comprehensive studies to uncover relations among structure and quantum properties of layered monochalcogenides will be carried out.

The undergraduate student will be involved on a project to generate the understanding needed to fully characterize monochalcogenide monolayers, novel 2D materials, a goal that will have repercussions in any new technology based from these quantum materials. This work will lead to a comprehensive understanding of the electronic, optical, spin, topological, and valley properties of these compounds. The specific questions to be addressed are: determining the atomistic process that triggers the transition from a *Pnma* onto a *Cmcm* phase in bulk layered phases; establishing the physics of valleytonics on monochalcogenide monolayers with a *Cmcm* structure at high temperature.

References (undergraduates appear highlighted):

SBL1: Two-dimensional disorder in black phosphorus and monochalcogenide monolayers. M. Mehboudi, **A.M. Dorio**, W. Zhu, A. van der Zande, H.O.H. Churchill, A.A. Pacheco-Sanjuan, E.O. Harriss, P. Kumar, and SBL. *Nano Lett.* **16**, 1704 (2016)

SBL2: Structural phase transition and material properties of few-layer monochalcogenides. M. Mehboudi, B. M. Fregoso, Y. Yang, W. Zhu, A. van der Zande, J. Ferrer, L. Bellaiche, P. Kumar, and SBL. *Phys. Rev. Lett.* **117**, 246802 (2016)

SBL3: Photostrictive two-dimensional materials in the monochalcogenide family. R. Haleoot, C. Paillard, M. Mehboudi, B. Xu, L. Bellaiche, and SBL. *Phys. Rev. Lett*. **118**, 227401 (2017).

SBL4: Intrinsic defects, fluctuations of the local shape, and the photo-oxidation of black phosphorus. **K.L. Utt**, P. Rivero, M. Mehboudi, E.O. Harriss, M.F. Borunda, A.A. Pacheco SanJuan, and SBL. *ACS Central Science* **1**,320 (2015).