Exploring 2D Materials for Novel Applications from First-Principles

Oğuz Gülseren*

Bilkent University, Department of Physics, 06800, Ankara, Turkey
**Corresponding Autor's Email: gulseren@fen.bilkent.edu.tr*

Abstract: Two-dimensional materials are expected to become key components for novel applications for not only electronic devices but also for energy storage applications including super capacitors and batteries because of their exotic properties. Fully understanding of most of material properties needs an atomistic description from quantum mechanics. In this respect, we present the investigation of several state-of-the-art 2D systems from first-principles calculations based on the density functional theory. Examples will include mechanical properties for friction of sliding of graphene or transition metal dichalcogenide layers, the electronic transport properties of the hybrid metallic-semiconducting lateral junctions formed between metallic (1T and 1Td) and semiconducting (2H) phases of MoS2, energy applications as high capacity anode material for battery and supercapacitors, peculiar piezoelectric properties of various 2D systems, and layered perovskites for solar cells [1-8].

Keywords**:** *2D materials, density functional theory, energy applications*

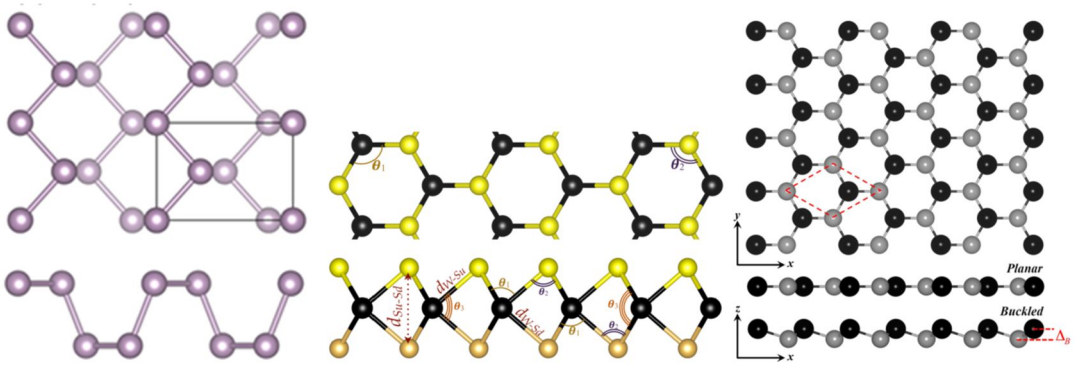

Fig. 1. Atomistic models of various 2D systems.

ACKNOWLEDGMENT: This work is supported by TUBITAK Project No: 115F024.

REFERENCES

[1] Y. Aierken, C. Sevik, O. Gülseren, F.M Peeters, D. Çakır, *J. Mater. Chem*. A, 2018, **6,** 2337-2345.
[2] T. Kocabaş, D. Çakır, O. Gülseren, F. Ay, N. K. Perkgöz, C. Sevik, *Nanoscale* 2018, **10**, 7803-7812
[3] Y. Aierken, C. Sevik, O. Gülseren, F.M Peeters, D. Çakır, *Nanotechnology* 2018, **29**, 295202.
[4] A. Mobaraki, A. Kandemir, H. Yapicioglu, O. Gülseren, C. Sevik, Computational *Mater. Sci.* 2018, **144**, 92–98
[5] C. Sevik, J. Wallbank, O. Gülseren, F.M. Peeters, D. Cakir, *2D Materials*, 2017, **4**, 035025
[6] M. Fadaie, N. Shahtahmassebi, M.R. Roknabad, Oğuz Gülseren; *Comput. Mater. Sci.* 2017, **137**, 208-214.
[7] C. Sevik, D. Çakır, O. Gülseren, F.M. Peeters; *J. Phy. Chem. C* **2016**, **120**, 13948-13953.
[8] D. Çakır, C. Sevik, O. Gülseren, F. M. Peeters; *J. Mater. Chem. A* 2016, **4**, 6029-6035.