Investigation of Optoelectronic Properties of 2D Materials by Ab Initio Methods

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The discovery of graphene has initiated a great volume of theoretical and experimental work regarding the exceptional mechanical, electronic and optical properties of two-dimensional (2D) materials, as well as their potential applications in technological advancement. Due to the increasing demand for 2D materials in applications such as display systems, LEDs, optical modulators and photovoltaics, the accurate calculation of the optical properties of 2D materials has become of great importance. In this respect, the main theme of this study is the use of ab initio calculations for the development of new emerging 2D materials through the identification of stable atomic structures, the investigation of crystal growth patterns and the calculation of the optoelectronic properties of the structures deemed promising following the initial screening [1,2]. In addition, we analyze the electronic and optical properties of functional hetero-materials [3]. The effect of doping/charging, stress-strain, number of layers and the excitonic effects are among the phenomena that we investigate. We utilize the state of the art computational methods to investigate a series of functional 2D structures for optoelectronic applications. These predictions regarding 2D structures of group V elements, group III-V compounds and hetero-systems may inspire experimental studies and contribute to the fundamental understanding.

[1] D. Kecik, E. Durgun, S. Ciraci, Phys. Rev. B 94, 205409 (2016)
[2] D. Kecik, E. Durgun, S. Ciraci, Phys. Rev. B 94, 205410 (2016)
[3] A. Onen, D. Kecik, E. Durgun, S. Ciraci, Phys. Rev. B 95, 155435 (2017)

Revealing the Origins of Friction via Atomic Force Microscopy

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Friction is a universal phenomenon that plays a major role in various technical processes. Despite its importance from both practical and scientific points of view, the fundamental physical principles that govern friction are not well-understood. In this talk, we will report recent results of friction experiments based on atomic force microscopy (AFM) from our laboratory at Bilkent University. In particular, the remarkable discovery of *structurally lubric* sliding (i.e., sliding with ultra-low friction theoretically expected between atomically-flat, molecularly-clean interfaces formed by two crystalline but incommensurate surfaces) exhibited by gold nano islands on graphite under ambient conditions will be introduced [1]. The talk will conclude with a discussion regarding the extension of structural lubricity to noble metals other than gold.

[1] E. Cihan, S. İpek, E. Durgun, M.Z. Baykara, *Nature Communications* **7**, 12055 (2016)