סמינריון

הנך מוזמן/ת להרצאה סמינריונית של הפקולטה להנדסת מכונות שתתקיים ביום ד' 24.02.21 (י"ב באדר, תשפ"א), בשעה 13:30 באמצעות הזום:

https://technion.zoom.us/j/95451172986

מרצה: גל אבירם

מנחה: פרופ'/ח דן מרדכי

על הנושא:

The Mechanical Interaction between Carbon-Nano Tubes and Graphene Sheets

The seminar will be given in Hebrew

תקציר ההרצאה :

Engineering materials with the ability to control the structure at the atomic level is the heart of modern technology. Devices based on stacked layers of graphene are candidates to form a new family of materials with unique properties, such as the superconductivity of twisted bilayer graphene. However, while most of the focus is paid to using stacks of 2D atomic structures, less attention is paid to the combination between carbon nanotubes (CNTs) (1D structures) and 2D material. In experiments performed recently in the group of Prof. Yaish from the Technion, it was found that when CNTs are deposited on graphene they deform diametrically, as opposed to when depositing them on quartz.

The main goal of this work is to perform a systematic computational study of the diametrical deformation of CNTs on graphene sheets, and how different parameters, such as orientation relation, size and defects, affect the interaction. Using molecular statics (MS) simulations, we generated a configuration of a single-wall CNT on a graphene sheet and the final shape of CNT was found from the relaxed configuration. We have found that for small diameters (below ~1.2nm) the CNT remained nearly cylindrical, whereas larger CNTs deformed and a contact between the CNT and the graphene sheet formed. The results were compared with an elastic continuum model, in which the CNT was considered as an elastic thin tube, which interacts with flat surface. The model, that was informed with values of the rigidity of the CNT and the interface energy from atomistic simulations, was in excellent agreement with the MS simulations. In addition, we show that the orientation relation has a small effect on the diametrical compression, rationalized with the values of the rigidity and the interface energy. Additionally, defects were introduced in the CNTs (either vacancies or Stone-Wales defects) and their effect on the diametrical deformation is discussed. Finally, the results are compared with the experimental findings and the possible differences are discussed.

בברכה,

פרופ"ח אתי סאס

מרכז הסמינרים