

## סמינריון

הנדך מוזמן/ת להרצאה סמינריונית של הפקולטה להנדסת מכונות שתתקיים ביום ב' 23.11.2020

(ז' בכסלו, תשפ"א), בשעה 14:30 באמצעות הזום :

<https://technion.zoom.us/j/95249776511>

**מרצה :** ליה טבי

**מנחה :** פרופ' ח דן מרדכי

**על הנושא :**

**תנודות של ננחוטס מתכתיים עם תרמוסטטים שונים בסימולציות דינמיקה מולקולרית**

### **Oscillations of metallic nanowires in molecular dynamics simulations with different thermostats**

The seminar will be given in Hebrew

**תקציר ההרצאה:**

In the recent years, there is an increasing interest to use nanowires as basic building blocks in mechanical and electronic devices. One of the ideas is to exploit their dynamic elastic properties to develop devices such as resonators and mass detectors. At this scale, atomistic simulations naturally capture the oscillations of metallic nanowires. However, one key issue is the loss of energy due to internal forces in the mechanical and electronic devices, which was not captured in atomistic simulations of nanowires. One possible solution proposed in literature is using a heat bath. In this study, we wish to examine if and how thermostats in molecular dynamics simulations affect the transverse-mode oscillations of metallic nanowires. We modeled penta-twinned nanowires in the canonical ensemble, i.e. the system does not conserve mechanical energy by coupling the nanowire to a heat bath, using two types of thermostats: Langevin and Nosé–Hoover (NH). We also examined two scenarios, in one the nanowire is continuously oscillated in the transverse direction and in the second case, it is clamped after a certain time of oscillations. The Langevin thermostat was found to strongly dissipate the oscillations in both scenarios. On the other hand, the NH thermostat demonstrated a decaying oscillation in the clamped case, which depends on the thermostat parameters. When continuously oscillating the nanowire with the NH thermostat, steady whirling motion is found in a range of frequencies near the resonance. The dependence on the thermostat parameters and a comparison with continuum theory is performed.

בברכה,

פרופ' ח דן מרדכי

מרכז הסמינרים