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| הפקולטה להנדסה כימיתע"ש וולפסון |  |  |
| The Wolfson Department of Chemical Engineering |  |  |

**Wolfson Department of Chemical Engineering Seminar**

**Thursday, November 25th, 2021 at 15:00**

**Via zoom <https://technion.zoom.us/j/97577956516>**

**From Observation to Design – Exploring the Combined Powers of Supervised Learning and Atomistic Simulations**

**Dr. Dan Mendels**

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 One of the key challenges facing computational molecular and material modeling is the simulation of systems and processes which characteristic time scales lie well beyond the reach of standard simulations. A central strategy to overcome this challenge has been to purposefully add artificial bias potentials to such systems in manners that effectively flatten their free energy landscapes and consequently lead to the  acceleration of their sampling by orders of magnitude. The manner by which these bias potentials are added is determined by so called collective variables (CVs), tailored specifically to suit any given problem. Constructing suitable CVs, however, can be a challenging task, one that has to date primarily relied on intuition and trial and error.

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In this talk, we will present a machine learning based method to systematically construct CVs. Despite the fact that the method requires as input little knowledge regarding a studied system, we show that its use in a variety of cases gives rise to very effective sampling. Additionally, exploiting the method’s interpretability and the notion that suitably constructed CVs compactly encode the essence of the slow transitions of studied systems, we propose their use as tools for engineering and demonstrate the idea on example cases.

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