מכון ויצמן למדע
WEIZMANN INSTITUTE OF SCIENCE

Thesis for the degree
Doctor of Philosophy

עבודת גמר (תזה) לתואר
דוקטור לפילוסופיה

Submitted to the Scientific Council of the
Weizmann Institute of Science
Rehovot, Israel

מוגשת למועצה המדעית של
מכון ויצמן למדע
רחובות, ישראל

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פיתוח מבוסס מחקר של יחידה קוריקולרית בתוכנית מדע חישובי בינתחומי

Statistical thermodynamics - Research-Based Development of a Curricular Unit in an Interdisciplinary Computational Science Program

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November 2020

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Abstract

This dissertation presents a research-based design of a 'statistical thermodynamics' curricular unit, which is part of a program "Introductory Computational Science: Chemical and Biological Physics" (ICS), intended for capable and interested high school students. This program focuses on physical modelling, both analytical and computational, of self-organization phenomena in interacting, multi-particle systems, that also have applications to chemistry and biology. It responds to the increasing demand for interdisciplinarity in science education, as well as for incorporating authentic scientific practices.

The design of the unit incorporates a novel organization of the teaching sequence and separates the traditional scheme of kinetic and potential energy that are usually taught and conceptualized together. Rather, kinetic energy is presented in the context of thermal contact and potential energy in the context of interparticle interactions – chemical binding and adsorption. This ordering overcomes conceptual framework changes and discontinuities (deterministic / stochastic) appearing in traditional curricula and allows a consistent learning progression to take place, all within the framework of multi-particle systems. The final projects of the students consisted of developing analytical and computational models of adsorption in simplified biological contexts, applying free energy minimization and Boltzmann probability respectively.

Empirical research was carried out in two contexts: Students' invoking and application of thermo-statistical concepts in solving thermal contact problems, carried out in a mid-year exam, and two case studies, constituting in-depth interviews regarding students' final projects. Findings from the mid-year exam indicated students largely invoked and applied various thermo-statistical concepts correctly, but also revealed students' tendency to assume entropy always increase, even for non-isolated systems. Findings from the end of year interviews demonstrated that one excelling student did indeed establish an operational framework of statistical thermodynamics with a robust knowledge organization; the student also exhibited ownership of both models they developed in the final project. The other student demonstrated more limited knowledge and a variety of alternative perceptions indicating a lack of progress in going from dynamical models and causal reasoning, to statistical ones. Our findings point at the extent of the programs' ability to transmit thermo-statistical understanding for some students, with effectively no incorrect perceptions, but also suggests the necessity for several modifications, most notably in externalizing the transition from dynamical to statistical models, which will improve the accessibility of the ICS to different students.