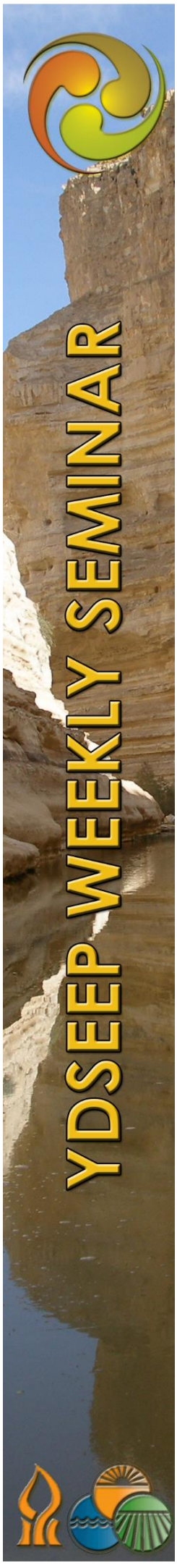

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Understanding Molecular and Hybrid Crystals from First Principles

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Abstract

Molecular crystals are crystalline solids composed of molecules bound together by relatively weak intermolecular interactions, typically consisting of van der Waals interactions and/or hydrogen bonds. Hybrid crystals combine molecular units and covalent/ionic networks. Both classes of crystals play an important role in many areas of science and engineering, ranging from biology and medicine to mechanics and electronics. Therefore, much effort has been dedicated to understanding their structure and properties

Predicting the behavior of such materials from first principles is highly desired for understanding their unique properties and for allowing rational design of novel materials and structures. Preferably, we would like to obtain such understanding from density functional theory (DFT), because the relative computational simplicity afforded by DFT allows us to attack realistic, experimentally accessible problems. Unfortunately, despite many other successes, DFT has traditionally struggled with useful prediction of properties of crystals that contain weakly-bound units.

Here, I will show how state-of-the-art DFT approaches allow us to overcome these limitations, quantitatively. I will focus on our recent progress in explaining and even predicting important classes of collective effects, i.e., phenomena that the individual units comprising the crystal do not exhibit, but arise through their interaction. Specifically, I will address unique structural, mechanical, electrical, and optical properties of both biogenic and synthetic crystals, with an emphasis on constructive interaction between theory and experiment.

Date & Location:

Tuesday, May 22, 2018, 11:00
Lecture room, Physics Building (ground floor)