Connecting Chemistry and Physics using Computational methods for Rational Materials Design

Ilya Grinberg
Department of Chemistry, Bar Ilan University

Computational methods play a key role in providing the microscopic-level understanding of the relationship between the material's composition, structure and properties. In this talk, I will discuss our recent computational studies of molecular electrocatalysts and ferroelectric perovskite oxides used for photovoltaic and non-volatile memory applications that reveal how chemistry and physics of the materials give rise to their desired functional properties. The understanding obtained in these studies is a step toward rational design of new materials.