Stony Brook University
The Graduate School

Doctoral Defense Announcement

Abstract

Simulating Complex Problems in Condensed Matter Physics:

from Liquid Water to Dark Matter-Electron Interactions

By

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Computational methods have been extremely useful in condensed matter physics by virtue of their capability to describe its complex many-body nature. Density functional theory has emerged as the predominant simulation framework to quantum-mechanically describe systems with low to intermediate correlation, from crystals to liquids to biomolecules. Due to its ubiquity and importance for life and technology, liquid water has concentrated research efforts since these methods were conceived. Nevertheless, challenges are still open in the study of this essential substance which has proven extremely difficult to simulate accurately. The fine interplay of hydrogen bonding, cohesive van der Waals forces and hydrogen delocalization through nuclear quantum effects results in a very complex scenario in which small microscopic errors result in great discrepancies with the observed macroscopic properties. In this thesis we compare the microscopic interactions with different energy density functionals, shedding light on how to improve them. We also study the microscopic structure of liquid water with machine learning methods, addressing the question of the existence of two coexisting microscopic molecular environments. Lastly, we apply density functional theory to study a completely different problem: the interaction properties of dark matter particles with electrons in semiconducting and scintillating crystals. Our calculations provide accurate theoretical quantifications that lay the first stone for the next generation of dark matter detectors, having the potential to detect this unobserved constituent of the universe and settle one of the greatest mysteries of fundamental physics.

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