

VISTA Seminar

Seminar 76

October 2, 2024

10:00 am – 11:30 am EDT / 3:00 – 4:30 pm BST London / 4:00 pm – 5:30 pm CEST Paris / 10 pm – 11:30 pm CST Beijing

TOC:

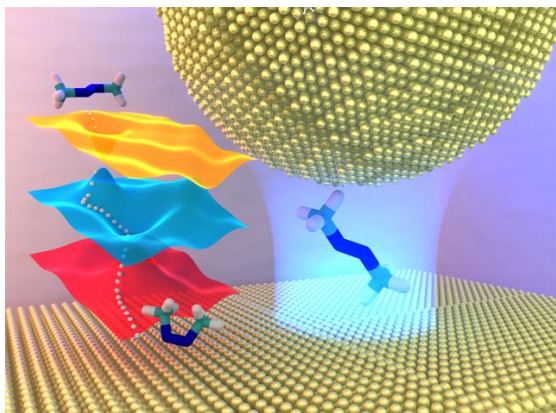
1. Presenter 1: Dr. Yu Zhang, Los Alamos National Laboratory, USA.....	page 2
2. Presenter 2: Dr. Martin van Horn, KTH Royal Institute of Technology, Sweden.....	page 3
3. How to connect.....	page 4

Light-Matter Hybridization and Entanglement from the First Principles

Yu Zhang

Theoretical Division, Los Alamos National Laboratory, Los Alamos, NM 87545, USA,

Email: zhy@lanl.gov



The intersection of quantum electrodynamics (QED) and molecular processes has yielded remarkable advancements in altering molecular properties and reactivity by exploiting light-matter couplings. As polaritonic states—hybrid electron-photon states—gain prominence in chemical applications, the need for understanding the underlying mechanisms of polaritons-mediated processes has stimulated the development of ab initio QED methodologies [1]. These advancements have led to the extension of many traditional electronic structure methods to molecular quantum electrodynamics framework, including Hartree-Fock (HF), Density Functional Theory, and Coupled-Cluster theories. In this talk, I will introduce variational transformation-based molecular quantum electrodynamics mean-field methods [2-3] designed to handle light-matter interactions across all coupling strengths and their importance in capturing electron-photon correlations and post-HF calculations. Additionally, I will present the quantum Monte Carlo (QMC) methods [4-5] for obtaining numerically exact solutions for polaritonic ground states. Our study reveals significant insights into electron-nuclear-photon interactions, such as shifts in the cavity Born-Oppenheimer surface minimum, wave function localization, and mode occupation, with results compared directly against state-of-the-art polaritonic coupled-cluster methods. Finally, I will discuss how to examine the quantum effect and light-matter entanglements from the principles, which would give more insights into the polariton-mediated phenomena beyond pure energy calculations.

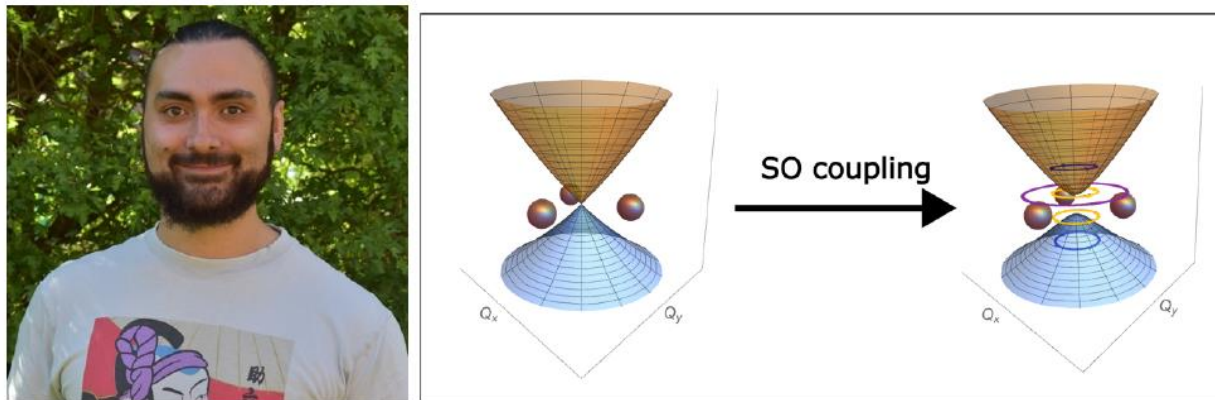
References:

1. B. M. Weight, X. Li, Y. Zhang, “Theory and modeling of light-matter interactions in chemistry: current and future”, *Phys. Chem. Chem. Phys.* 25, 31554 (2023).
2. X. Li, Y. Zhang, “First-principles molecular quantum electrodynamics theory at all coupling strengths”, arXiv:2310.18228
3. Ilia Mazin, Y. Zhang, “Variational Squeezing States and Light-Matter Entanglement from the First Principles”, in preparation.
4. B. M. Weight, S. Tretiak, Y. Zhang. “Diffusion quantum Monte Carlo approach to the polaritonic ground state”, *Phys. Rev. A.*, 109, 032804 (2024).
5. B. M. Weight, Y. Zhang. “Auxiliary Field Quantum Monte Carlo with Gaussian Ansatz for Light-Matter Interactions”, in preparation.

An Electronic Spin on Geometric Phase Effects in Molecular Systems

Martin van Horn and Nanna Holmgaard List

KTH Stockholm. Email: martinvh@kth.se



Molecules are inherently geometric in nature, as their properties are not only determined by their atomic composition but also their three-dimensional arrangement in space. However, the geometry arising from the atomic configuration alone is rather mundane, essentially being given by a tuple of Cartesian coordinates. A more exotic type of geometry emerges from the interplay between the nuclear coordinates and the electronic wave function. It is known, for instance, that the electronic wave function may not return to its initial state when transported around a closed contour in nuclear coordinate space, with the difference given by a phase factor.[1] This phase factor is geometric in nature only depending on the path taken in nuclear coordinate space and bearing some resemblances to the notion of curvature in Riemannian manifolds. When the nuclear motion is treated quantum mechanically according to the Born-Oppenheimer approximation, the geometric phase translates to an effective vector potential describing a pseudo-magnetic interaction with the nuclei. It can be argued that interactions of this type are most relevant if the electronic wave function is complex-valued, which, for instance, occurs if there is a conical intersection or if spin-orbit coupling is included.[2] Using a simple triatomic toy-model that exhibits a conical intersection at equilateral configuration, I will illustrate why geometric phase effects necessarily occur under these conditions. In addition, the results presented in this talk will be formulated using fibre bundles, providing a mathematical yet approachable perspective to the geometric phase effect.

References:

- [1] M. V. Berry, *Proc. R. Soc. Lond. A* **1984**, 392, 45-57.
- [2] A. C. Mead, *Chem. Phys.* **1980**, 49 (1), 33-38.

How to connect

Alexey Akimov is inviting you to a scheduled Zoom meeting.

Topic: VISTA, Seminar 76

Time: Oct 2, 2024 10:00 AM Eastern Time (US and Canada)

Join Zoom Meeting

<https://buffalo.zoom.us/j/91832490081?pwd=Dybgde1mYPgbBedDbeeTFiKBylr9jL.1>

Meeting ID: 918 3249 0081

Passcode: 601275