Building a multi-ion mixed-qudit-boson simulator for quantum chemistry

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Mixed-qudit-boson (MQB) simulators [1] are versatile platforms for studying quantum systems that involve both discrete and continuous degrees of freedom. By combining qudits, bosonic modes, and efficient coupling between them, they can enable simulations outside regimes where classical methods excel. This is particularly relevant in chemistry, where MQB simulators allow the study of phenomena beyond the Born-Oppenheimer approximation. An iconic example is conical intersections, which play a fundamental role in various chemical processes, including the very first step in the process of human vision [2].

While individual conical intersections have been successfully simulated on trapped-ion MQB simulators [3,4] using only single qubits, modelling more realistic energy landscapes requires scaling up to accommodate a larger number of electronic states and vibrational modes. This can be realised using an ion-chain in a linear Paul trap, which we have built at PSI. In this poster, we present our latest advancements, focusing on individual addressing with crossed AODs and spatially resolved readout using a fast camera.

[1] MacDonell, R. J. et al. Analog quantum simulation of chemical dynamics. Chem. Sci. 12, 9794-9805 (2021).
[2] Sen, S. and Deupi, X. Study of Photoselectivity in Linear Conjugated Chromophores Using the XMS-CASPT2 Method. ACS Phys. Chem Au 4, 736-749 (2024).
[3] Valahu, C. H. et al. Direct observation of geometric-phase interference in dynamics around a conical intersection. Nat. Chem. 15, 1503-1508 (2023).
[4] Whitlow, J. et al. Quantum simulation of conical intersections using trapped ions. Nat. Chem. 15, 1509-1514 (2023).