Small polarons in solid state systems by first principles

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Polarons are quasiparticles arising from the coupling of excess electrons or holes with ionic vibrations in polarizable materials, and they have a profound impact on material properties and functionality [1]. The role of polarons in materials can be investigated at the microscopic level using atomistic simulations based on density functional theory, and recent advances, particularly the integration of machine-learning techniques, have significantly expanded the scope and accuracy of these ab initio approaches.

In this seminar, we will discuss several examples of polaron-mediated phenomena in transition-metal oxides, where theoretical predictions are supported by a variety of spectroscopic, optical, and transport measurements. These include: (i) hole bipolarons as precursors of the superconducting state in doped BaBiO3 [2]; (ii) electron polaron formation and dynamics at TiO2 surfaces [3, 4]; and (iii) spin-orbit polarons acting as inhibitors of a Mott transition in the double perovskite Ba2NaOsO6 [5].

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