Symmetry-based Floquet optical selection rules help explain light-induced sidebands

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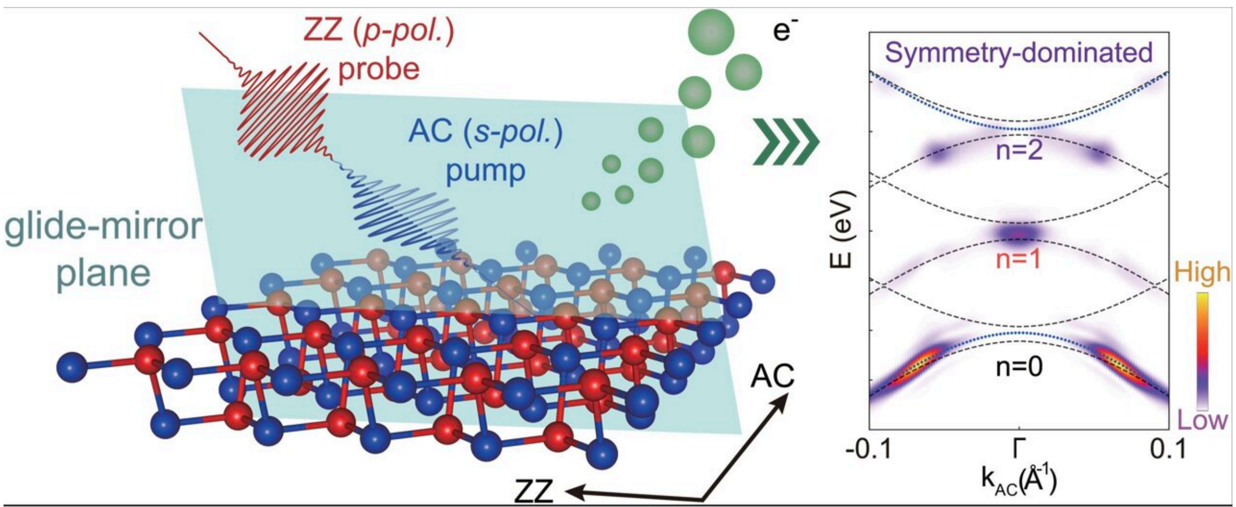

Disentangling spectral weight distributions in TrARPES via Floquet optical selection rules. Credit: Max Planck Society

Researchers at the Max Planck Institute for the Structure and Dynamics of Matter (MPSD), in collaboration with international partners, have developed momentum-resolved Floquet optical selection rules. They show how these symmetry-based rules determine the spectral weight distributions of photon-dressed sidebands in time- and angle-resolved photoemission spectroscopy (TrARPES) experiments across different pump-probe configurations. This fundamental work has now been published in *Science Advances*.

Ultrafast lasers have revolutionized the control of electronic properties of quantum materials. When materials are subjected to strong periodic laser fields, their electronic states can hybridize with photons to form Floquet states. These states appear as transient, light-induced sidebands with distinct spectral weight distributions, which can be observed in TrARPES experiments.

Such nonequilibrium spectral features provide direct insights into the microscopic mechanisms of light-matter interactions in quantum materials, and are of central importance for advancing ultrafast photoemission spectroscopy and the engineering of Floquet band structures.

Yet, a critical challenge persists: although some experiments reveal that the detectability of these sidebands depends on the light polarization, a comprehensive theoretical explanation of these observations has been unsuccessful. This limitation has hindered the systematic design of photon-dressed states in quantum materials, a problem that this study successfully addresses.

"We find that the visibility of these sidebands follows symmetry-governed Floquet optical selection rules, similar in spirit to electric dipole transitions in equilibrium induced by an external light field," explains lead author Benshu Fan, postdoctoral researcher at the MPSD.

Hannes Hübener, research group leader at the MPSD, adds, "Our framework systematically connects the symmetries of the material, the pumping and probe lasers, as well as the Floquet index to determine whether sidebands can appear under specific pump-probe conditions."

The research team chose monolayer black phosphorus (BP), a layered semiconductor with a highly anisotropic crystal structure, as a prototypical system. They validate these selection rules through state-of-the-art ab initio time-dependent density functional theory (TDDFT) simulations. These simulations reproduce known experimental phenomena of Floquet engineering in the BP thin film. They additionally predict new spectral features under unexplored geometries, all of which are naturally explained by the newly discovered Floquet optical selection rules.

"These results show the power of symmetry in explaining and predicting light-induced phenomena," says Peizhe Tang, professor at the Beihang University and guest scientist at the MPSD.

Notably, the researchers extended their approach beyond monolayer BP, demonstrating its transferability to other materials such as hexagonal boron nitride. This extends the reach of Floquet engineering to a wider class of materials and experimental setups.

Angel Rubio, Director of the MPSD's Theory Department, concludes, "This framework will be an essential tool for engineering symmetry-controlled non-equilibrium quantum states, paving the way for future Floquet engineering in ultrafast spectroscopy."

More information: Benshu Fan et al, Floquet optical selection rules in black phosphorus, *Science Advances* (2025). DOI: 10.1126/sciadv.adw2744

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