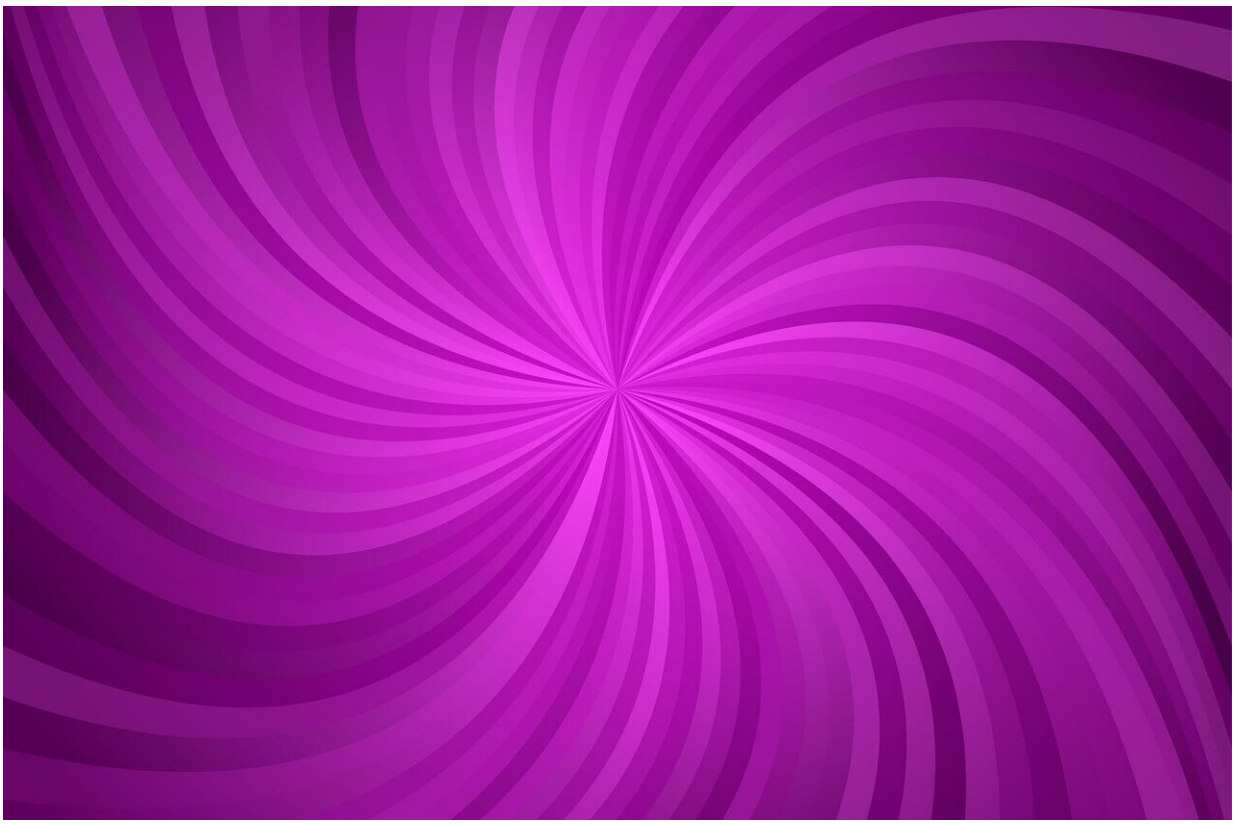
Scientists realize real-time GW-BSE investigations on spin-valley exciton dynamics

March 25 2021



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Prof. Zhao Jin's research team from University of Science and Technology of China (USTC) has made important progress in the

development of spin-valley exciton dynamics. The research developed an ab initio nonadiabatic molecular dynamics (NAMD) method based on spin-resolved exciton dynamics. The team gained the first clear and complete physical picture of valley exciton dynamics in MoS_2 from the perspective of first-principles calculations based on GW plus real-time Bethe-Salpeter equation (GW + rtBSE-NAMD).

The method can accurately include many-body effects at the level of first principles and break through the bottleneck of GW+BSE method in time-dependent dynamics. The research results were published in *Science Advances*.

From investigations on MoS_2, the research provides a comprehensive picture of spin-valley exciton dynamics where the electron-phonon (e-ph) scattering, spin-orbit interaction (SOI), and electron-hole (e-h) interactions come into play collectively.

In this work, the team develop an ab initio NAMD method based on GW plus real-time propagation of BSE (GW + rtBSE-NAMD). The SOI is included by using the spinor basis sets, and the e-ph coupling is simulated by combining ab initio MD (AIMD) with real-time BSE. The team used the rigid dielectric function approximation and used GW + rtBSE-NAMD to investigate the spin-valley exciton dynamics in monolayer MoS_2.

It was found that the intervalley bright exciton transition induces fast valley depolarization within a few picoseconds, which provide direct evidence that e-h exchange interaction plays an essential role in the intervalley bright exciton transitions in TMD systems.

The newly developed GW + rtBSE-NAMD method provides a powerful tool to investigate time- and spin-resolved exciton dynamics. This method can also be widely applied to other material systems to study

important physical problems such as exciton relaxation, lifetime, dissociation, and interaction with defects, opening the door to the field of exciton dynamics in solid materials based on first principles.

More information: Xiang Jiang et al, Real-time GW-BSE investigations on spin-valley exciton dynamics in monolayer transition metal dichalcogenide, *Science Advances* (2021). DOI: 10.1126/sciadv.abf3759

Provided by University of Science and Technology of China