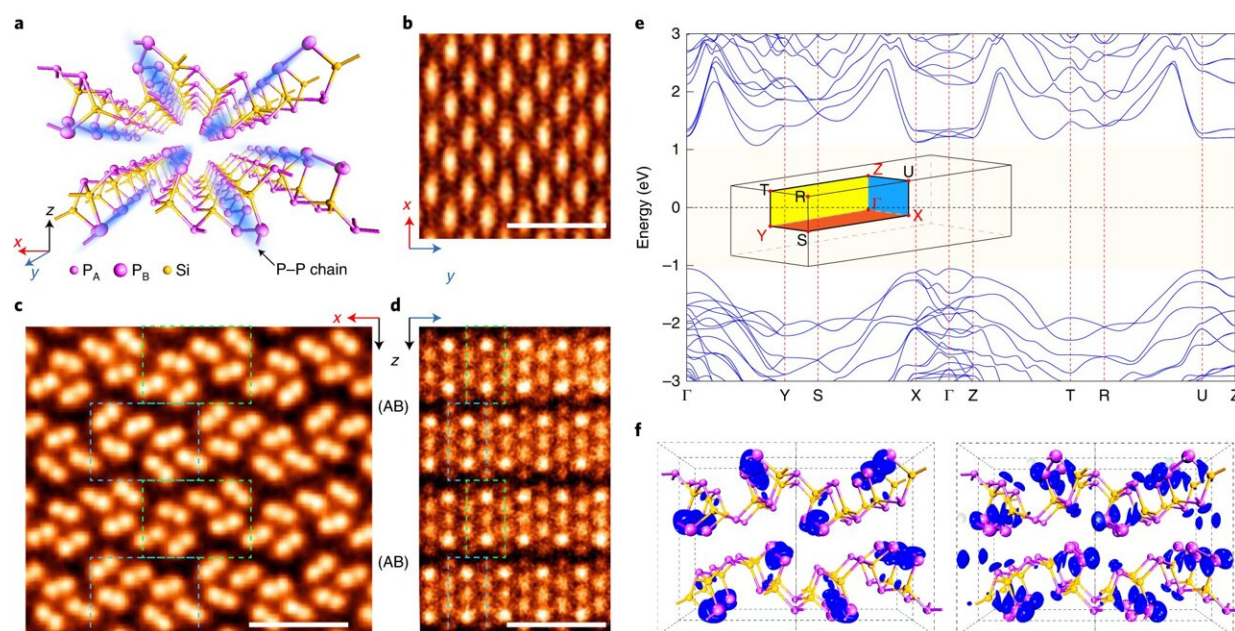


# New class of excitons with hybrid dimensionality in layered silicon diphosphide

June 20 2022, by Jenny Witt



Crystal structure and band structure of layered  $\text{SiP}_2$ . **a**, Schematic layered structure of  $\text{SiP}_2$  ( $Pnma$ , group number 62). The  $x, y, z$  coordinate system is defined according to the crystal structure, as shown in the bottom-left corner. The blue shading highlights the  $\text{P}_B\text{--P}_B$  chains formed by the  $\text{P}_B$  atoms along the  $y$  direction of the crystal lattice, which play a critical role in generating quasi-1D electronic and excitonic states. **b–d**, Top view (**b**) and cross-sectional (**c,d**) STEM–ADF images of  $\text{SiP}_2$  viewed along the  $y$  axis (**c**) and  $x$  axis (**d**). Green and cyan dashed rectangles represent the periodic lattice with ABAB stacking order of  $\text{SiP}_2$  layers. Scale bars, 1 nm. **e**, Electronic band structure of bulk  $\text{SiP}_2$  calculated from the  $GW$  method. The inset shows the first BZ of bulk  $\text{SiP}_2$ .  $\text{SiP}_2$  is a semiconductor with an indirect band gap of 2.14 eV. The valence band maximum is at the  $\Gamma$  point, and the conduction band minimum is located along

the  $\Gamma$ -Y direction. The conduction band minimum state does not contribute to the formation of the A exciton due to the large direct interband transition energies at this location. **f**, Charge density distribution of the conduction band edge (left) and valence band edge (right) in real space. The isosurface of the plot is  $0.02 \text{ e } \text{\AA}^{-3}$ . Credit: *Nature Materials* (2022). DOI: 10.1038/s41563-022-01285-3

Researchers from Nanjing University and Beihang University in China and the Max Planck Institute for the Structure and Dynamics of Matter (MPSD) in Hamburg, Germany, have produced a new class of exciton with hybrid dimensionality by engineering the properties of layered silicon diphosphide ( $\text{SiP}_2$ ). Their work has been published in *Nature Materials*.

Excitons are bound particles that consist of a negatively charged electron and a positively charged electron hole. Their exotic behavior offers an important new platform to study the physics of materials when they are coupled to other states of matter, such as vibrations of the material's [crystal lattice](#).

Using  $\text{SiP}_2$ , researchers in China fabricated a new kind of material whose 2D layers are bound by van der Waals forces and feature strong internal covalent interactions. This produces peculiar one-dimensional phosphorus chains along which electronic states can localize. The team then managed to engineer a new kind of exciton with hybrid dimensionality in this layered material, meaning that the electron has a 1D character and the hole displays 2D characteristics. This is the first time such a phenomenon has been observed. Theoreticians at the MPSD confirmed the findings with advanced simulations.

By exposing the material to [laser light](#), the experimentalists were able to

create and subsequently probe these excitonic states, which appear as peaks in the measured spectra. In particular, the emergence of a peculiar side peak to the main excitonic peak in the spectra shows a distinct signature of the hybrid dimensionality excitons: Due to their strong dependence on the material's internal structure, the newly-created excitons are expected to interact strongly with other material excitations, such as lattice vibrations that alter the phosphorous chains in  $\text{SiP}_2$ .

The theory group at the MPSD subsequently confirmed these findings through extensive analysis, using state-of-the-art methods to investigate the excitonic particles. Their simulations show that the particle consists of a positively charged hole with 2D character and a negatively charged electron that is localized along the 1-dimensional phosphorous chains, giving rise to excitons with mixed dimensionality.

The theoreticians demonstrated that such an exciton interacts strongly with lattice vibrations, which generates the experimentally measured side peak feature. Such a feature has so far only been measured in low-dimensional materials such as graphene nanotubes or transition metal dichalcogenide monolayers, but not in a [bulk material](#) such as  $\text{SiP}_2$ .

This collaboration has shown the existence of [exciton](#)-phonon sidebands in a 3D bulk crystal as well as excitonic states with hybrid dimensionality. With scientists looking for new ways to control and investigate the interactions between quasi-particles such as excitons, phonons and others in solid materials, these findings represent important progress.

"Our approach provides an intriguing platform to study and engineer new states of matter such as trions (two electrons and one hole or vice versa) and more complex particles with hybrid dimensionality," says co-author Peizhe Tang, Professor at Beihang University and visiting scientist at the MPSD.

Fellow co-author Lukas Windgätter, a doctoral student in the Institute's Theory group, adds: "To me it is intriguing how one can control the interactions of particles through engineering solids. Especially being able to create composite particles with hybrid dimensionality opens up pathways to investigate new physics."

**More information:** Ling Zhou et al, Unconventional excitonic states with phonon sidebands in layered silicon diphosphide, *Nature Materials* (2022). [DOI: 10.1038/s41563-022-01285-3](https://doi.org/10.1038/s41563-022-01285-3)

Provided by Max Planck Institute for the Structure and Dynamics of Matter

Citation: New class of excitons with hybrid dimensionality in layered silicon diphosphide (2022, June 20) retrieved 10 April 2024 from <https://phys.org/news/2022-06-class-excitons-hybrid-dimensionality-layered.html>

<p>This document is subject to copyright. Apart from any fair dealing for the purpose of private study or research, no part may be reproduced without the written permission. The content is provided for information purposes only.</p>
--