I. Physikalisches Institut (IA)
Phasenwechselmaterialien
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Topic for a Bachelor/Master Thesis

„Orbital-resolved design of novel materials for universal memory and photonic computing“

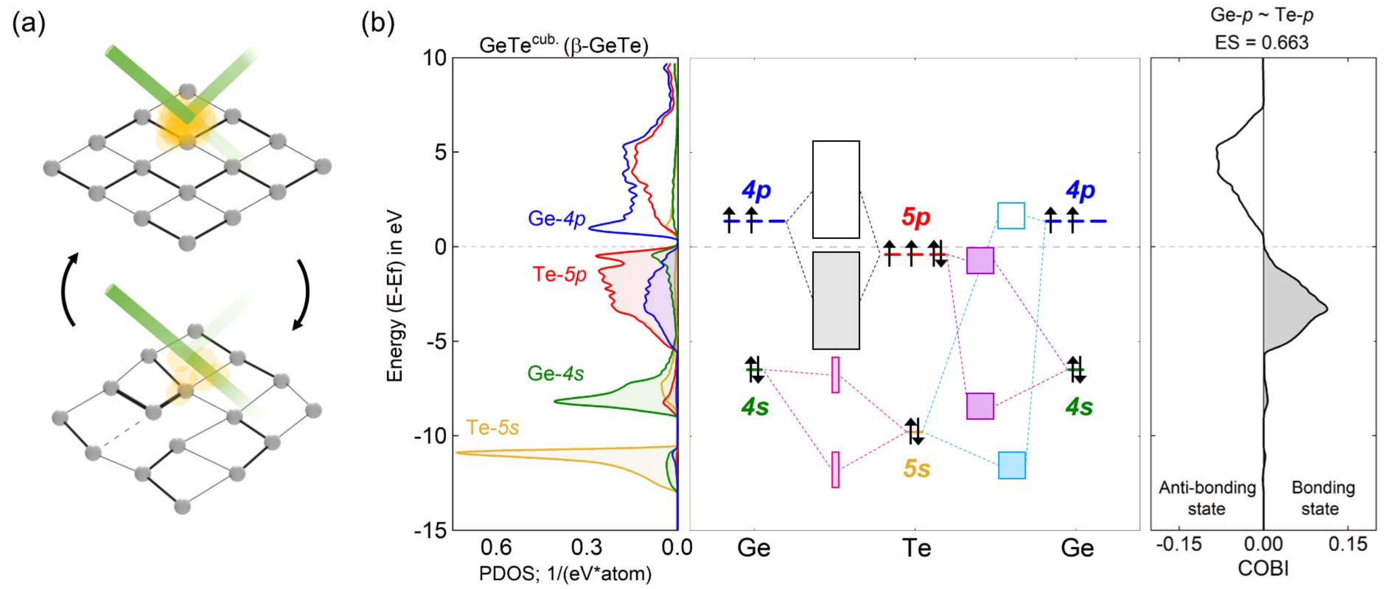

Figure 1. (a) Electrical/optical contrast depending on the degree of orbital alignment. (b) Orbital-resolved density of states and interactions between orbitals.

Drastic generation of free carriers (yellow in **Figure 1a**) depending on the orbital alignment becomes one of the most promising bases of universal memory and photonic computing, which revolutionizes Von Neumann architecture by reducing to the limit of latency. [1] Over the past five years, our group has successfully implemented a framework that characterizes chemical bonding by the number of shared and transferred electrons (ES and ET), enabling us to verify and predict exotic properties of the optimized materials such as GeTe. [2] This framework is particularly effective for systems lacking atomic ordering, where conventional band structure theories are not applicable. [3]

We are currently extending the framework characterizing bonding from real-space to energy-space to study contributions between orbitals. As shown in **Figure 1b**, orbitals are deconvoluted in partial density of states (PDOS; left panel) and interactions between them are plotted in crystal orbital bond index (COBI; right panel) that molecular orbital picture can be available (central panel). Based on these achievements, we look forward to study the mechanisms behind the drastic generation of free carriers and establish design principles for faster, more energy efficient, and longer-lifespan materials.

[1] *Nat. Rev. Mater.* **2019**, 4, 150-168.
[2] *Adv. Mater.* **2021**, 33, 2102356
[3] *Proc. Natl. Acad. Si. U.S.A* **2024,** 121, e2316498121

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