



Münchner Physik- Kolloquium

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Metavalent bonding in solids: provocation or promise?

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Scientists and practitioners have long dreamt of designing materials with novel properties. Yet, a hundred years after quantum mechanics lay the foundations for a systematic description of the properties of solids, it is still not possible to predict the best material in applications such as photovoltaics, superconductivity or thermoelectric energy conversion. This is a sign of the complexity of the problem, which is often exacerbated by the need to optimize conflicting material properties. Hence, one can ponder if design routes for materials can be devised.

In recent years, the focus of our work has been on designing advanced functional materials with attractive opto-electronic properties, including phase change materials, thermoelectrics, photonic switches and materials for photovoltaics. Phase Change Materials have provided a special challenge for materials optimization. They possess a remarkable property portfolio, which includes the ability to rapidly switch between the amorphous and crystalline state. Surprisingly, in PCMs both states differ significantly in their properties. This material combination makes them very attractive for applications in rewriteable optical and electronic data storage, as well as photonic switches. In this talk, the unconventional material properties will be attributed to a unique bonding mechanism (metavalent bonding). Further evidence for this bonding mechanism comes from a quantum-chemical map, which separates the known strong bonding mechanisms of metallic, ionic and covalent bonding. The map reveals that metavalent bonding is a new, fundamental bonding mechanism. This insight is subsequently employed to design phase change as well as thermoelectric materials. Yet, the discoveries presented here also force us to revisit the concept of chemical bonds and bring back a history of vivid scientific disputes about 'the nature of the chemical bond'.

