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## Combining computational design and soft synthesis to a resource efficient green chemistry of novel functional materials

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**Statement of the Problem:** Megatrend developments from digitalisation to environmental challenges and the scarcity of resources drive an increasing need for new materials. They should be smart, low dimensional (from 3D to 2D and nano size) and highly functional – Phosphorene is a good example. Materials and their processing should also be "green" and resource efficient. This causes a still puzzling question to find the "right" material within the large number of possible combinations of chemical elements from a systematic approach.

**Methodology & Theoretical Orientation:** We report on the combination of soft experimental chemistry and computational materials design within the phase diagram A-M-Ch. First, we focus on main group metals A like Phosphorous (P) [1, 2] and Phosphorene allotropes with a systematical understanding of structures and properties. Next we ask for the understanding and design of ternary materials like helical SnIP [3], pyrites MACh, and half perovskites $AM_{3/2}X$ [4,5].

Findings: From our cooperative work phosphorene like $P_xA_{1-x}$ and helical SnIP were recently described as smart 2D and 1D semiconductors with tunable band gaps. Within ternary A-M-X compounds superconducting parkerites and shandite like $Sn_2Co_3S_2$ and became a highly fascinating 2D system for spintronic, thermodynamic and skyrmionic properties. From computational chemistry and experiment a rational design to tune specific properties upon substitution could be reached. Further a guided synthesis could be reached by predicting stable and metastable compositions and structures. With the scheme of energy diagrams formation and decay of compositions as well as the formation of competing products are predicted. Novel results on new 3D and 2D materials are presented, that are reached by novel soft and conversion synthesis.

**Conclusion & Significance:** the combination of modern computational and synthetic inorganic chemistry leads an efficient way to green materials design.

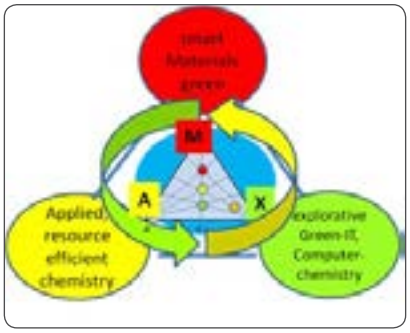


**Figure 1.** Combination of green and applied ressource efficient computer and experimental chemistry.

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3. B. Liu, M. Köpf, A. A. Abbas, X. Wang, Q. Guo, Y. Jia, F. Xia, R. Weihrich, F. Bachhuber, F. Pielnhofer, H. Wang, R. Dhall, S. B. Cronin, M. Ge, X. Fang, T. Nilges, C. Zhou, Black Arsenic-Phosphorus: Layered Anisotropic Infrared Semiconductors with Highly Tunable Compositions and Properties, Adv. Mater 2015, 27, 4423-29.
4. R. Weihrich, W. Yan, J. Rothballer · Ph. Peter, S. M. Rommel, S. Haumann, F. Winter, Ch. Schwickert, R. Poettgen, Tuneable anisotropy and magnetism in Sn2Co3S2–xSex – probed by 119Sn Mößbauer Spectroscopy and DFT studies, Dalton Trans., 2015, 44, 15855 – 15864.
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**Biography**

Richard Weihrich is professor for chemistry of materials and resources (CMR) at the institute of materials resource management (MRM) of the University of Augsburg, Germany. He studied chemistry in Regensburg with Diploma, PhD and habilitation thesis. Therein he developed the combined use of methods of experimental and theoretical chemistry to discover and to exploit novel materials.

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**Notes:**