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Encapsulation of inorganic nanoparticles into novel *T. maritima* encapsulin variants

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Encapsulation of inorganic nanoparticles into novel *T. maritima* encapsulin variants

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Supported by an established synthetic strategy towards optical materials protein containers and nanoparticles are used. With protein containers as building blocks, nanoparticles will be assembled with high precision into mesoscale materials with optical properties that emerge from interactions between the components. Along the recent advances in computational redesign of protein containers, it is now possible to combine these results with nanoparticle synthesis and protein crystallography. An innovative design approach with two oppositely charged protein containers as building blocks, a new type of protein-based material will be realized (Figure 1). Surface charged protein containers can be combined with inorganic compounds to unite biological features with the chemical and physical properties of abiotic materials. In particular, protein containers, with their inherent ability to encapsulate cargo molecules, are perfect platforms for the generation of multifunctional assemblies.[1, 2] Gold nanoparticles can be decorated with a small number of encapsulin cargo-loading peptides to fill protein containers. By lock-and-key interaction between the peptides and the peptide-binding pockets on the inner container surface (Figure 2), the nanoparticles will be encapsulated with high efficiency.[3] Typically encapsulin bears a flavin that is attached to the outer surface. The flavin leads to a yellow coloured solution and its presence on the protein surface might be problematic for future applications or in crystallization. Based on the latest cryo-EM data it was possible to remove the flavin.[4] Crystalline materials are produced, which is crucial for future applications. Because the protein scaffold is independent of the nanoparticle cargo, this modular approach will enable tuning of the optical properties by choice of nanoparticle content, assembly type and protein container type. For further future applications, surface charged protein containers will be used as sustainable building blocks for bioinorganic nanomaterials.[5]

References:

- [1] M. Künzle, T. Eckert, T. Beck J. Am. Chem. Soc. 2016, 138, 12731.
- [2] M. Lach, M. Künzle, T. Beck Chem. Eur. J. 2017, 23, 17482.
- [3] M. Künzle, J. Mangler, M. Lach, T. Beck Nanoscale 2018, 10, 22917-22926.
- [4] D. Diaz et al. bioRxiv 2020, preprint
- [5] M. Lach, M. Künzle, T. Beck, Biochemistry 2019, 58, 140-141.

Figure captions:

Figure 1: Strategy overview for the synthesis of highly structured optical nanomaterial.

Figure 2: Gold nanoparticle encapsulation via cargo-loading peptide into *T. maritima* encapsulin.

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