Masters / Bachelor thesis opportunities 2022

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Various opportunities are available to conduct a research project towards a Bachelor or Masters degree with a focus on ceramic materials and processing.

If any of the below themes interests you and you are interested in conducting an engaging and multi-faceted world-class research project towards a Bachelor or Masters degree during 2022, please contact me at dorian.hanaor@ceramics.tu-berlin.de to see how you can apply your skills and inquisitiveness towards high value outcomes in this topic.

Sodic orthosilicates Na_2MSiO_4 as cathodes in sodium ion batteries

There is tremendous interest in sodium-ion batteries (NaIBs) as an approach to address large scale energy storage challenges, which pose the biggest obstacle in the ongoing energy transition, from fossil fuels to renewables. Sodium ion batteries are of interest in large scale energy storage as alternatives to Lithium-ion batteries, as sodium is more terrestrially abundant than Li and such batteries are generally considered safer than Li based systems. A significant challenge in the development of new NIBs, is the development of effective cathode materials that allow efficient cyclical intercalation and release of Na^+ ions with minimal polarization barriers, and without requiring the use of toxic or scarce raw materials.

Sodic orthosilicates have been investigated with a view towards NIB cathode materials. Such cathode materials offer the possibility of cheaper large-scale batteries that would enable the rapid deployment of significant storage capacity, without depending on scarce or expensive raw materials. Sodic orthosilicates have the general form **Na_2MSiO_4**, where M generally represents a cation in a +2 oxidation state. As orthosilicates offer broad ranges of substitution, diverse candidates for M have been studied, mainly relating to transition metals Fe, Mn, Co and Ni. In such materials, sodium layers are separated by transition metal oxide layers. Minimising Jahn-Teller distortion in TMO layers is key to enabling reversible intercalation of sodium ion into the cathode material and is governed by cation speciation and distribution in these layers. In addition the performance of the cathode material is affected by its topology and microstructure. In cathode materials a balance of ionic and electronic conductivity, along with high levels of intercalation sites is generally achieved through a heterogeneous granular structure combining electronic and ionic conduction phases.

In this work the student will investigate methods for the synthesis of homogenous sodic orthosilicates in nanocrystalline phases, by soft chemistry method and examine how processing and composition affect cation distribution. To ascertain the relationship between processing of materials performance, half-cell electrochemical characterisation will be conducted in representative battery tests. This project will develop new knowledge and insights relating to processing-performance relationships in sodium ion batteries.

Machine learning based design of silicates with low thermal expansion

Machine learning is emerging as a key technology for the predictive design of high performance materials across a broad range of applications. In parallel the field of mm wave dielectrics is gaining significant momentum as high frequency devices become widespread in 5G technology and the internet of things. In the context of wireless data transmission in the millimetre wave range, the important characteristics are, naturally, optimal dielectric properties but also low thermal

expansion and high thermal conductivity to allow for easy integration in e.g. hard ceramic substrate applications as well as good heat dissipation [1]. Silicate materials have been identified as a class of materials that can combine all these properties, as they are already well studied in terms of low permittivity and high quality factors towards implementation into prospective high frequency dielectric applications.
Promising thermal expansion behaviour has been observed for some alkali earth orthosilicates such as Ba2SiO4, Sr2SiO4, or Ca2SiO4 [2]. Further, a near zero coefficient of thermal expansion (CTE) has also been found for the compound HfSiO4 [3]. Inspired by this, and with a view towards gleaning a better understanding of the origins of these phenomena, here at Fachgebiet Keramische Werkstoffe we used deep learning techniques based on CrabNet to generate direct predictions of the thermal expansion coefficient as well as uncertainty in Nesosilicates.

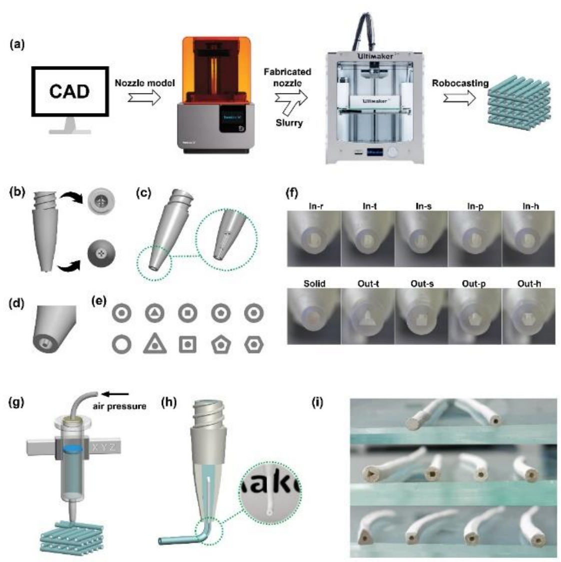
In this project the student will experimentally examine thermal expansion in silicate ceramics based on $TiSiO_4$ and together we will gain deeper insights into the design of future mm wave dielectric materials with optimised physical properties.

This project is suitable for those who have some initial experience and familiarity with Python and Machine Learning.
[1] M. L. Minges, Electronic Materials Handbook: Packaging, ASM International, 1989, vol. 1, pp. 334–335.
[2] J. Tony and M. T. Sebastian, Mater. Lett., 2010, 65, 891.
[3] Varghese, Jobin, et al. Dalton Transactions 44.11 (2015): 5146-5152.

Bone-tissue-Engineering: Additive manufacturing and sintering of Hollow Strut polycrystalline silicate ceramic scaffolds

A recent capability developed at Fachgebiet Keramische Werkstoffe relates to the fabrication of hollow strut scaffolds. These scaffolds offer advantages in terms of specific strength, bioactivity and transport, making it possible to achieve higher performance in bone-tissue engineering scaffolds.

In this project the student will gain experience implementing a brand-new 3D printing method for state- of the art bioceramics based on materials with the composition $Sr_xCa_{1-x}Cu_yMg_{1-y}Si_2O_6$. The focus of the research will be to determine the role of processing, specifically sintering, structure and composition on the mechanical and biological performance of these novel bone scaffolds.



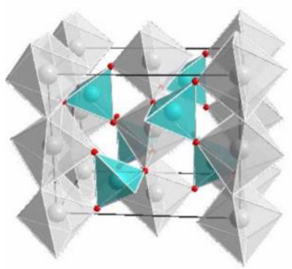
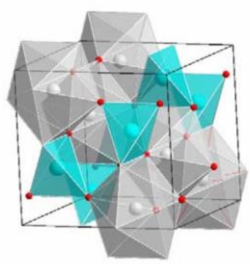
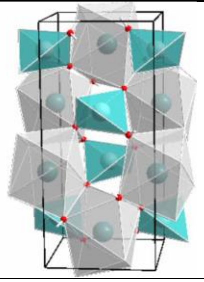
Synthesis of forsterite ceramics by soft-chemistry methods

Forsterite, Mg2SiO4, is a commonly occurring member of the olivine group of silicate minerals. As a functional ceramics, forsterite shows significant untapped potential. Utilising forsterite in applications as dielectrics requires the ability to synthesis this material in dense and highly pure forms. Currently reported synthesis methods do not allow the formation of dense, single phase forsterite without the use of very high temperatures. In this work we will explore cation substitution and soft chemistry synthesis as a pathway towards reducing densification temperatures and minimising the formation of secondary phases, specifically enstatite, in the processing of this interesting mineral inspired ceramic.

Processing, polymorphism and performance of $TiSiO_4$ ceramics

Titanium silicate is an interesting silicate material that has not yet been fully explored as a ceramic in terms of its potential towards low-thermal expansion materials and high performance dielectrics. Interestingly this phase exhibits polymorphism with three known phases occurring. The formation and transformations between these phases merit further investigation. In this project we will examine the Sol Gel synthesis of $TiSiO_4$ and examine its formation in the metastable Zircon-type phase. We will examine the substitution of Ti with other cations and consider how this affects densification, polymorphism and performance

The thermal expansion of the material will be examined by dilatometry. Dielectric performance will be studied in the mm wave spectrum, with implications towards utilisation in 5G communication systems and automotive radar.

	$CrVO_4$	**Zircon**	**Scheelite**
Crystal structure of $TiSiO_4$	orthorhombic Cmcm	tetragonal $I4_1/amd$	tetragonal I41/a
			
density	3.4396 g/cm^3	3.9255 g/cm^3	4.2757 g/cm^3
Permittivity	4.46 – 5.55	3.59 – 4.43	4.78 – 5.88

Synthesis and characterisation of high entropy oxides

High entropy ceramics present an interesting class of materials whereby a single crystalline phase is stabilised by the presence of a large number of cations at equivalent sites. Here at TU Berlin we have developed polymer based methods for the fabrication and additive manufacturing of high entropy oxides. In this project the research student will further develop and adapt these methods for the processing of high entropy perovskites. The functionality of these materials as lithium ion battery anodes will be tested as will other functional properties including permittivity and fracture toughness. In this project in a relatively short time frame, we will gain significant new knowledge and insights relating to the processing-performance relationships in high entropy perovskite materials.