I-4 Prevention in construction-from the molecule to the structure

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ABSTRACT

Buildings of the infrastructure are subjected to various environmental impacts, which often lead to the failure of materials and structures. In this context the capillary uptake of aqueous solutions containing chlorides or sulfates, is crucial for the duration of the repair-free service life. A well-established method to prevent these transport processes is the use of water repellent treatments carried out with silicon organic compounds like silanes. However, the development of construction chemicals, which include the group of silanes used for the preventive protection of concrete, are still based on more or less empirical approaches. Because of that the reliability of water repellent treatments is in many cases insufficient, often the application already failed after a few years. Frequently, the causes for this were unknown and led to a loss of confidence in this technology. In recent years' modern methods of computational chemistry, e.g. based on the Density Functional Theory (DFT) have been increasingly used to analyze the chemical behavior of the silanes in the presence of cement-based materials in order to establish structure-effect relationships. With these methods we are be able to design new water repellent agents targeted with well-defined properties. This contribution presents these methods and shows exemplarily their application for the development of a newly gel-based hydrophobing agent. Additionally, with selected cases it will be shown how these scientific methods help to improve the effectiveness and durability of applications in practice.