

In Silico Materials Design (ISIMADE) and experimental validation for novel optical coatings

Scientific Summary

The objective of this project is to develop advanced pragmatic modeling tools to conduct and accelerate the design and development of optical thin film coatings and integrate that design capability with the strength of the Flemish materials industry. *The environment to perform some materials design "in silico" is right.* The recent decade has witnessed the high usefulness of computer experiments as a practical research tool in condensed matter. The systematically increasing capabilities of computer simulations have actually reached such a high degree of accuracy that more and more they are employed for the design of new materials of high technology and practical use. The applicant team will focus on two important problems in computational materials modeling and will apply them to specific problems that are technologically relevant for the Flemish materials industry. A substantial emphasis will be given to the *prediction of structure* as it is the corner stone to rational materials design, and set of diverse skills will be brought together on this problem. The vision of the applicants is that the construction of a reliable platform for structure prediction is prerequisite for an accurate reproduction of electronic properties. In this project the applicants focus on *optical properties* of coatings as they form the keystones for many applications of interest to the Flemish industry: e.g. transparent conducting oxides (TCOs), coloured oxide coatings, etc. In order to fulfil the requirement of disposing of a methodology applicable to a broad range of materials problems, optical properties will be calculated with a variety of methods.

The final goal of this project lies in the design of new tailor made materials: the ability to design new materials with the desired optical properties. To achieve this goal existing computational tools will be improved on their efficiency and new concepts will be developed tailored to the specific needs as discussed above. In this way, new materials will be proposed by use of advanced computational tools after which they will be validated with experimental work.