Center for Molecular Modeling

K. Lejaeghere, K. Rijpstra
M. Sluydts, J. Jaeken
Prof. M. Waroquier
Prof. V. Van Speybroeck
Prof. S. Cottenier

Spectroscopy

Biochemistry & Organic Chemistry

Chemical Kinectics

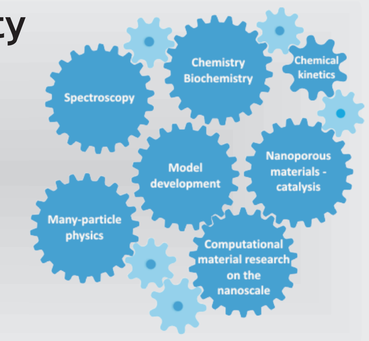
Material Physics

Many-Body Physics

Model Development

Nanoporous Materials

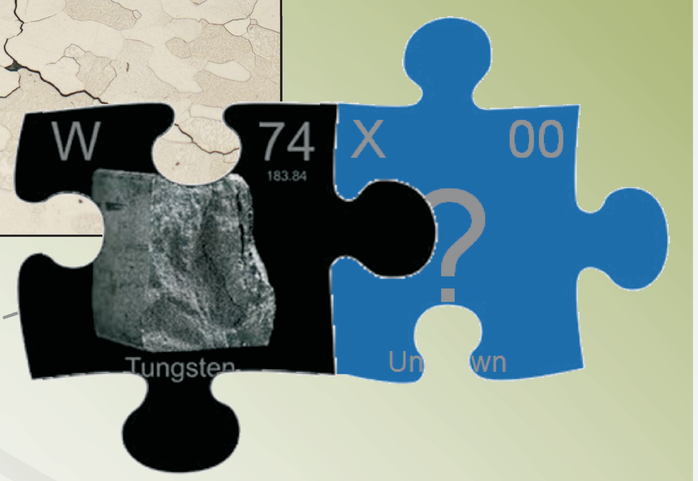
The Center for Molecular Modeling (CMM) is an interdisciplinary and interfaculty research center at Ghent University, developing and applying simulation methods in the fields of (bio)chemistry, applied physics and materials science.
This poster presents two case studies of ongoing research at the CMM within the context of 'materials for energy'.

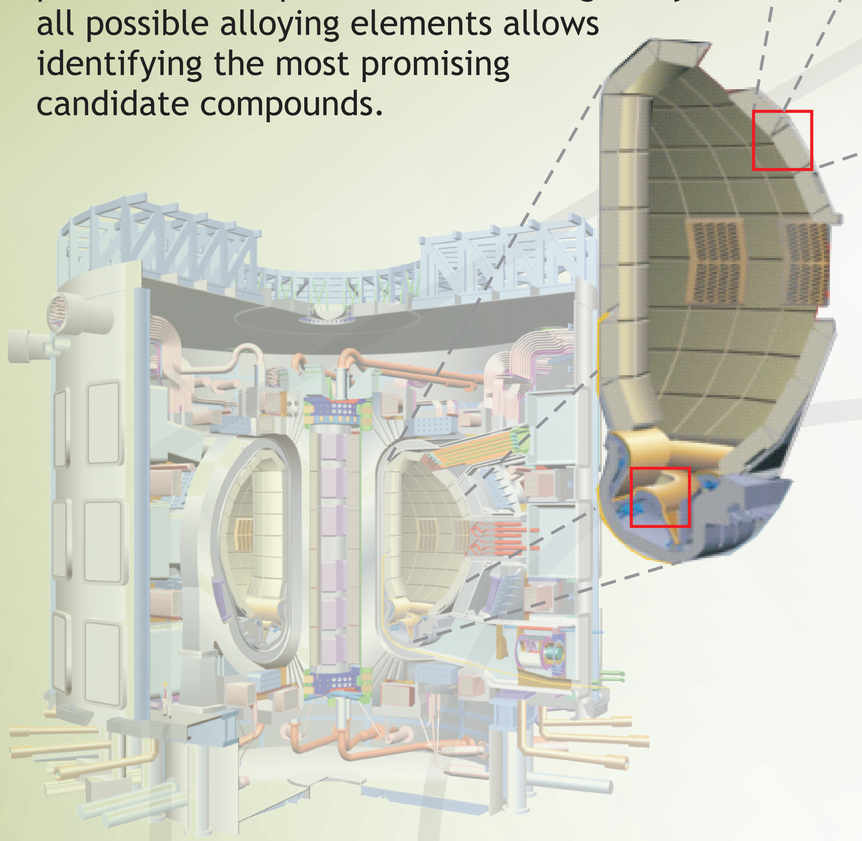


Materials for Energy: The Role of Computational Materials Design

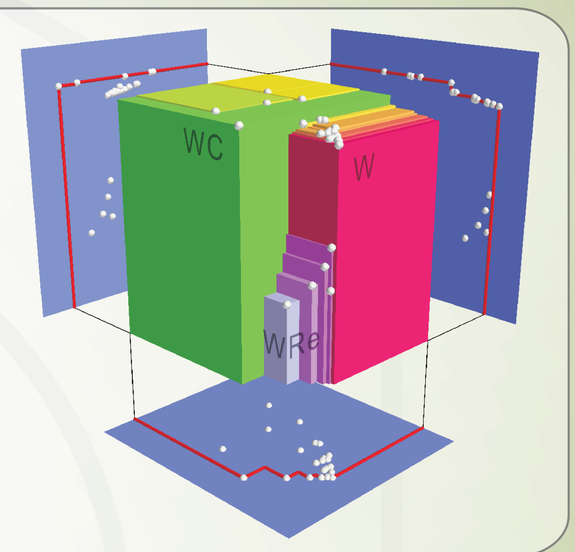
Structural materials for future fusion reactors

Materials in future fusion reactors will have to withstand harsh operating conditions, such as large neutron fluxes and high temperatures. This is particularly critical for the components which come into contact with the plasma. Tungsten offers the most promising perspectives, but is brittle at the relevant conditions. Alloying is one way to resolve this problem. A computational screening study of all possible alloying elements allows identifying the most promising candidate compounds.





Using data mining concepts, such as Pareto optimality, the most optimal W-alloys can be identified. Here, a 3D example is shown where price, hardness and thermal resistance are simultaneously optimized.



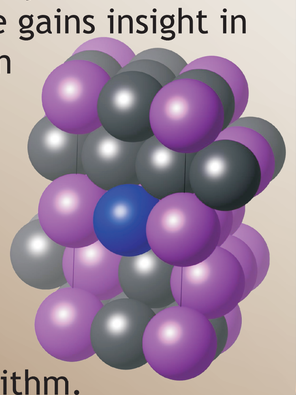
Safety assessment for future fission reactors

In the future MYRRHA reactor at SCK•CEN, the radiotoxic element polonium will always be present in the lead-bismuth eutectic (LBE) coolant due to transmutation of the latter two elements. Good knowledge on the interaction of this element with its surroundings is a prerequisite for the safety licensing of the installation.

Computational materials physics offers the unique chance to 'experiment' with such dangerous materials. It allows us to study the interactions between Po and its environment, narrowing down the area in which experimentalists have to look. This can drastically reduce the number of expensive and time-consuming experiments one has to perform.

Po in solid LBE

Does Po mind being in LBE?
By studying a variety of local environments, one gains insight in Po's preferences in a PbBi-alloy.

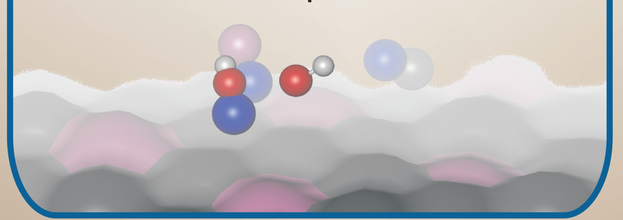


More ordered structures can be found using an evolutionary algorithm.

Po in gas phase

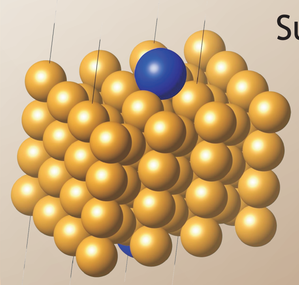
Po is likely to evaporate from the LBE and bind itself to smaller atoms in the atmosphere above.

With quantum mechanical calculations the formation probability of Po-containing molecules can be predicted.



Po adsorption on noble metals

In order to capture the evaporated Po, as element or in a molecule, the correct filter material has to be selected.



Surface calculations allow us to study the adsorption of Po-containing molecules on candidate filter materials.

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